Access DB# 84811

SEARCH REQUEST FORM

Scientific and Technical Information Center

| Mail Box and Bldg/Room Location: | umber 30 <u>5-0788</u> <u>CP3 11D30</u> Resul box CP3-11D0, | Serial Number: 09/935 7 ts Format Preferred (circle): (FAPER) D | |
|---|---|--|--|
| Include the elected species or structures, ke | ywords, synonyms, acrony hat may have a special mea | s specifically as possible the subject matter to b ms, and registry numbers, and combine with th ning. Give examples or relevant citations, auth bstract. | e concept or |
| Title of Invention: <u>UGHT-E</u> | MITTING DEVIC | CE AND MATERIAL TIL | CREOF |
| Inventors (please provide full names): | HISASHI OKA | ADA, TOSHIHIRO ISE | |
| MASAYUKI MISHIR | NA, TOSHICI | TAGUCHZ | |
| Earliest Priority Filing Date: | 2000-2541 | 71 (8/24/2000) Also 20 | 01-038718 CZ/*1. O1-236419(8)o1 |
| | | arent, child, divisional, or issued patent numbers) o | |
| | | 7 | |
| Please broade | n seinch (4 | um attached premi | n's |
| | sombilities _ | 1 7 (From the claim |) language, |
| search) to ally | of compour | om attached preve d D. From the claim we thought you u | rould be |
| | | interested in the | polymer - Kralatad |
| Clf nothing is | found for | compound D prie | |
| 8/24/2000 ple | ase also s | earch attached of | the abstracts |
| | | al C | e) attached |
| Compound | E plus a | tacked) | owever.) |
| | | | |
| thank y | on | | · |
| | · | | |
| | | | : |
| | ; | | į |
| | • . • . | | |
| ****** | ****** | ************ | ***** |
| STAFF USE ONLY | Type of Search | Vendors and cost where applicable | क्षण्यात्र का अपेता के कि |
| Searcher: | NA Sequence (#) | stn | |
| Searcher Phone #: | AA Sequence (#) | Dialog : | ······································ |
| Searcher Location: | Structure (#) | Questel/Orbit | |
| Date Searcher Picked Up: | Bibliographic Litigation | | |
| Searcher Prep & Review Time: | Litigation | Lexis/Nexis Sequence Systems | |
| | | | |

Other

Online Time:

PTO-1590 (8-01)

10

or a substituent; n^E and m^E each independently represent an integer of 0 to 5; and n' represents 0 or 1.

9. The light-emitting device according to claim 1, wherein
5 the heterocyclic compound is a polymer comprising a repeating unit represented by formula (E):

$$(R_{i-1}^{E1})_{nE_{o-5}}$$

$$(R_{i-1}^{E2})_{nE_{o-5}}$$

$$(R_{i-1}^{E2})_{mE_{o-5}}$$

$$(E)$$

wherein Ar^E represents an arylene group or a divalent heterocyclic group; R^{E1} and R^{E2} each independently represent a hydrogen atom or a substituent; n^E and m^E each independently represent an integer of 0 to 5; and n' represents 0 or 1.

20 10. The light-emitting device according to claim 9, wherein the substituent is a group selected from the group consisting of an alkyl group, an alkenyl group, an alkynyl group, an aryl group, an alkoxy group, an aryloxy group, an acyl group, a halogen atom, a cyano group, a heterocyclic group, 25 and a silyl group.

$$(R^{D1})_{n^D}$$

wherein Ar Drepresents an arylene group or a divalent heterocyclic group; R^{D1} and R^{D2} each independently represent a hydrogen atom or a substituent; n^D represents an integer of 0 to 3; and m^D represents an integer of 0 to 5.

6. The light-emitting device according to claim 1, wherein the heterocyclic compound is a polymer comprising a repeating 20 unit represented by formula (D):

$$\begin{array}{c}
\begin{pmatrix}
H & H_2 \\
C & C
\end{pmatrix} \\
\begin{pmatrix}
Ar^D \\
N
\end{pmatrix} \\
N
\end{array}$$

$$\begin{pmatrix}
R^{D2} \\
M
\end{pmatrix} \\
\begin{pmatrix}
R^{D1} \\
N
\end{pmatrix} \\
\begin{pmatrix}
R^$$

25

wherein Ar^D represents an arylene group or a divalent heterocyclic group; R^{D1} and R^{D2} each independently represent a hydrogen atom or a substituent; n^D represents an integer of 0 to 3; m^D represents an integer of 0 to 5; and m' represents 0 or 1.

- 7. The light-emitting device according to claim 6, wherein the substituent is a group selected from the group consisting of an alkyl group, an alkenyl group, an alkynyl group, an aryl group, an alkoxy group, an aryloxy group, an acyl group, a halogen atom, a cyano group, a heterocyclic group, and a silyl group.
 - 8. A polymer comprising a repeating unit represented

SEARCH REQUEST FORM

Scientific and Technical Information Center

| Requester's Full Name: DAWN GARRETT Examiner #: 76107 Date: 1/16/2003 |
|---|
| Art Unit: 1770 Phone Number 30 5 - 0 1/8 8 Serial Number: 09/935 /// |
| Mail Box and Bldg/Room Location: CP3 -11D30 Results Format Preferred (circle): PAPER DISK E-MAIL (or Mailbox CP3 - 11D03) |
| If more than one search is submitted, please prioritize searches in order of need. |
| ************************************** |
| Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract. |
| Title of Invention: LIGHT-EMITTING DEVICE AND MATERIAL THEREFOR |
| Inventors (please provide full names): HISASHI OKADA, TOSHIHIRO ISE, MASAYUKI MIS |
| TOSHIKI TAGUCHI |
| Earliest Priority Filing Date: $\frac{7P}{2006-254171} \left(\frac{8}{24}/200\right)$, $\frac{7P}{7P} = \frac{2001-038718}{236419} \left(\frac{2}{8}\right)$ |
| *For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the |
| Please search attached compound (D) used in |
| Please search attached compound (D) used in a light-emitting (electroluminescent) denie |
| ArD is an anylene group |
| RDI and RDZ are hydrogens |
| $n^{\mathcal{D}}$ is 3 |
| m ^D is 5 |
| m' is l |
| |

=> file reg

```
FILE 'REGISTRY'
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2003 American Chemical Society (ACS)
=> d his
    FILE 'LREGISTRY'
1د
                STR
    FILE 'REGISTRY'
,2
              SCR 2043
              0 S L1 AND L2
    FILE 'LREGISTRY'
               STR L1
    FILE 'REGISTRY'
5
             0 S L4 AND L2
6
             0 S L4
    FILE 'LREGISTRY'
7
               STR L4
   FILE 'REGISTRY'
3
            0 S L7 AND L2
            13 S L7
LO
           365 S L7 FUL
               SAV L10 GAR401/A /
11
             6 S L10 AND PMS/CI
   FILE 'CAOLD'
.2
             0 S L11
   FILE 'ZCAPLUS'
.3
            1 S L11
   FILE 'HCAPLUS'
            1 S L11
5
           13 S L10
        79141 S LIGHT?(2A)(EMIT? OR EMISSION?) OR LED/IT OR L(W)E(W)D O
7
            1 S L15 AND L16
8
            1 S L14 OR L17
9
       498597 S PHOSPHORES? OR LUMINES? OR FLUORES?
0
            1 S L15 AND L19
            1 S L14 OR L17 OR L18 OR L20
   FILE 'REGISTRY'
```

<EP G1=(0-1) CY
IODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
</pre>

RAPH ATTRIBUTES: ≷ING(S) ARE ISOLATED OR EMBEDDED ∜UMBER OF NODES IS 18

14

STEREO ATTRIBUTES: NONE 10 365 SEA FILE=REGISTRY SSS FUL L7

100.0% PROCESSED 6290 ITERATIONS 3EARCH TIME: 00.00.01 365 ANSWERS

=> file hcaplus FILE 'HCAPLUS' JSE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

=> d 121 1 ibib abs hitstr hitind

L21 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS ACCESSION NUMBER: 2002:354001 HCAPLUS

DOCUMENT NUMBER: 136:377202

TITLE: Light-emitting device and

Garrett 09/935,711

material therefor

Okada, Hisashi; Ise, Toshihiro; Mishima, IVENTOR(S):

Masayuki; Taguchi, Toshiki

Fuji Photo Film Co., Ltd., Japan ATENT ASSIGNEE(S): U.S. Pat. Appl. Publ., 91 pp.

CODEN: USXXCO

CUMENT TYPE:

Patent

ANGUAGE:

)URCE:

English

AMILY ACC. NUM. COUNT:

ATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|----------|----------------------|------------------|----------|
| | | | | |
| US 2002055014 JP 2002319491 RIORITY APPLN. INFO. | A1 A2 | 20020509 20021031 | US 2001-935711 | 20010824 |
| | | | JP 2001-236419 | 20010803 |
| | | | | 20000824 |
| | • | | | 20010215 |
| | | | JP 2001-236419 А | 20010803 |

THER SOURCE(S):

MARPAT 136:377202

Light-emitting devices comprising a pair of electrodes formed on a substrate and org. compd. layers comprising a light-emitting layer provided in between the electrodes are described in which .gtoreq.1 of the org. compd. layers comprises a heterocyclic compd. having .gtoreq.2 atoms and a phosphorescent compd.; polymers with repeating units described by the general formulas I and II (Ar = arylene or divalent heterocyclic group; R1 and R2 = independently selected H or substituent; n = 0-3; q = 0-5; and m = 0-5), which may be employed as the heterocyclic compds. in the devices, are also described. The devices may also employ polymers of heterocyclic compds. from which AR is absent. The phosphorescent compd. may be an org.

=> file reg FILE 'REGISTRY' ENTERED AT 17:23:01 ON 22 JAN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 21 JAN 2003 HIGHEST RN 479664-17-0 DICTIONARY FILE UPDATES: 21 JAN 2003 HIGHEST RN 479664-17-0

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details: http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d his

L5

(FILE 'HOME' ENTERED AT 15:52:21 ON 22 JAN 2003)

FILE 'REGISTRY' ENTERED AT 16:02:42 ON 22 JAN 2003 ACT GAR401/A

L1 STR
L2 365 SEA FILE=REGISTRY SSS FUL L1
-----L3 6 S L2 AND PMS/CI
L4 359 S L2 NOT L3

_ _ _ _ _ _ _ _ _

FILE 'ZCA' ENTERED AT 16:03:40 ON 22 JAN 2003 13 S L4

FILE 'LREGISTRY' ENTERED AT 16:19:15 ON 22 JAN 2003 L6 STR

FILE 'REGISTRY' ENTERED AT 16:31:31 ON 22 JAN 2003

FILE 'HCA' ENTERED AT 16:39:40 ON 22 JAN 2003

L13 5 S L11

L14 116 S L12

L15 73619 S EL OR E(W)L OR (ELECTRO OR ORG# OR ORGANO#)(2A)LUM!N? O

L16 482050 S FLUORES? OR PHOSPHORES? OR LUMINES?

L17 28 S L14 AND (L15 OR L16)

L18 27 S L17 NOT L13

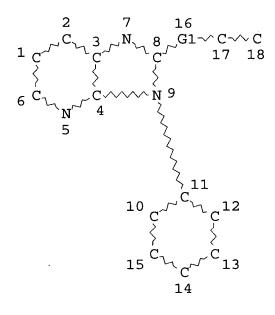
FILE 'LCA' ENTERED AT 16:43:39 ON 22 JAN 2003

FILE 'ZCA' ENTERED AT 16:43:55 ON 22 JAN 2003

FILE 'REGISTRY' ENTERED AT 17:23:01 ON 22 JAN 2003

=> d 14 que stat

L1 STR



REP G1=(0-1) CY NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 18

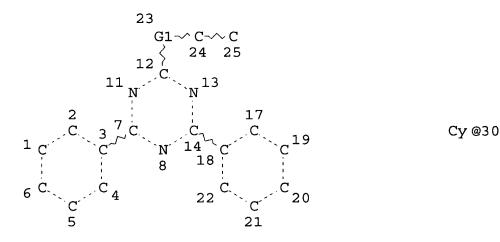
STEREO ATTRIBUTES: NONE

L2 365 SEA FILE=REGISTRY SSS FUL L1
L3 6 SEA FILE=REGISTRY L2 AND PMS/CI
L4 359 SEA FILE=REGISTRY L2 NOT L3

=> d l10 que stat

L8

STR



REP G1=(0-1) 30 NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM GGCAT IS UNS AT 30 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 22

STEREO ATTRIBUTES: NONE

L10

301 SEA FILE=REGISTRY SSS FUL L8

100.0% PROCESSED 5503 ITERATIONS

SEARCH TIME: 00.00.01

301 ANSWERS

=> file zca FILE 'ZCA' ENTERED AT 17:23:35 ON 22 JAN 2003 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2003 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 16 Jan 2003 VOL 138 ISS 4 FILE LAST UPDATED: 16 Jan 2003 (2003.0116/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 15 1,4-13 cbib abs hitstr hitrn

L5 ANSWER 1 OF 13 ZCA COPYRIGHT 2003 ACS

136:377202 Light-emitting device and material therefor. Okada, Hisashi; Ise, Toshihiro; Mishima, Masayuki; Taguchi, Toshiki (Fuji Photo Film Co., Ltd., Japan). U.S. Pat. Appl. Publ. US 20020055014 A1 20020509, 91 pp. (English). CODEN: USXXCO. APPLICATION: US 2001-935711 20010824. PRIORITY: JP 2000-254171 20000824; JP 2001-38718 20010215; JP 2001-236419 20010803.

GI

Light-emitting devices comprising a pair of electrodes formed on a substrate and org. compd. layers comprising a light-emitting layer provided in between the electrodes are described in which .gtoreq.1 of the org. compd. layers comprises a heterocyclic compd. having .gtoreq.2 atoms and a phosphorescent compd.; polymers with repeating units described by the general formulas I and II (Ar = arylene or divalent heterocyclic group; R1 and R2 = independently selected H or substituent; n = 0-3; q = 0-5; and m = 0-5), which may be employed as the heterocyclic compds. in the devices, are also described. The devices may also employ polymers of heterocyclic compds. from which AR is absent. The phosphorescent compd. may be an org. metal complex.

IT 422574-61-6P

(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle deriv. polymers for them)

RN 422574-61-6 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-(4-ethenylphenyl)-3-phenyl- (9CI) (CA INDEX NAME)

IT 422574-61-6P

(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle deriv. polymers for them)

L5 ANSWER 4 OF 13 ZCA COPYRIGHT 2003 ACS

Preparation of heterocyclic beta-3 adrenergic receptor Ashwell, Mark Anthony; Solvibile, William Ronald (American Home Products Corporation, USA). PCT Int. Appl. WO 2002006235 A1 20020124, 64 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-US22366 20010716. PRIORITY: US 2000-PV218700 20000717. This invention provides A-U-CH(OH)CH2NHCH2CH2VC6H4W-p (1) or a AB pharmaceutically acceptable salt thereof, which are useful in treating or inhibiting metabolic disorders related to insulin resistance or hyperglycemia (typically assocd. with obesity or glucose intolerance), atherosclerosis, gastrointestinal disorders, neurogenic inflammation, glaucoma, ocular hypertension and frequent urination; and are particularly useful in the treatment or inhibition of type II diabetes. .beta.3-Adrenergic receptor EC50 and maximal response (IA; % activity compd./% activity isoproterenol) values are reported for 16 example compds., e.g. 0.057 .mu.M and 1.12 for 3-[4-[2-[(2S)-2-hydroxy-3-(4hydroxyphenoxy)propylamino]ethyl]phenyl]-1-isopropenyl-1,3dihydroimidazo[4,5-b]pyridin-2-one. In 1, A is (a) a 5-6 membered heterocyclic ring having 1-4 heteroatoms selected from O, N, and S, substituted with (R1)m; (b) a Ph ring substituted with (R1)m; (c) a naphthyl ring substituted with (R1)m; or (d) a Ph fused heterocycle selected from (R1)m-substituted 1,3-dihydro-2-oxo-2H-benzimidazol-4yl, 1,3-benzodioxol-5-yl, 1,2,3,4-tetrahydro-2-oxoquinolin-5-yl, 1,2,3,4-tetrahydro-1-naphthylideneamino. U is -OCH2- or a bond; V is O or a bond; W is an amino or amido group wherein the N is substituted by an optionally substituted pyridyl or pyrazinyl ring

or the N is incorporated into an imidazole ring fused with a

pyridine or pyrazine ring. R1 is alkyl of 1-8 C atoms, aryl of 6-10 C atoms, -OR7, cycloalkyl of 3-8 C atoms, halogen, cyano, trifluoromethyl, CO2R7, NHCOR7, NHSO2R7, -NR7CONR8R9, -NR7R8, alkenyl of 2-7 C atoms, S(0) vR7, NO2, -O(CH2) uCO2R7, -OCONR7R8, -O(CH2)sOR7, or a 5-6 membered heterocyclic ring contg. 1 to 4 heteroatoms selected from O, S, and N. R2, R4, R7, R8, and R9 are each, independently, H, alkyl of 1-8 C atoms, aryl of 6-10 C atoms, cycloalkyl of 3-8 C atoms, or arylalkyl having 1-8 C atoms in the alkyl moiety; R3 is H, nitro, halogen, or -NR10R11. R5 is H; alkyl of 1-8 C atoms; alkenyl of 2-7 C atoms; arylalkyl having 1-8 C atoms in the alkyl moiety; alkyl of 1-8 C atoms, substituted with 1-4 substituents selected from -OR7 and halogen; -(CH2)qCR12R13(CH2)rR7; aryl of 6-10 C atoms, optionally mono, di, or trisubstituted with a substituent selected from halogen, cyano, nitro, trifluoromethyl, alkyl of 1-8 carbons optionally substituted with 1-4 substituents selected from OR7 or halogen, cycloalkyl of 3-8 C atoms, aryl of 6-10 C atoms, -NHCONR7R8, and -CO2R7; or a 5-6 membered heterocyclic ring contg. 1 to 4 heteroatoms selected from O, S, and N, which is optionally mono- or disubstituted with halogen, alkyl of 1-8 C atoms, or arylalkyl having 1-8 C atoms in the alkyl moiety. R6 is H, alkyl of 1-8 C atoms, alkenyl of 2-7 C atoms, or arylalkyl having 1-8 C atoms in the alkyl moiety; R10 and R11 are each, independently, H, alkyl of 1-8 C atoms, arylalkyl having 1-8 C atoms in the alkyl moiety, -COR7, or -CONR7R8; R12 and R13 are each, independently, H, alkyl of 1-8 C atoms, or aryl of 6-10 C atoms which is optionally substituted with alkyl of 1-8 C atoms or halogen; or R12 and R13 are taken together to form a spiro fused cycloalkyl ring of 3-8 C atoms. M = 0-2; q = 0-5; r = 0-5; s = 1-4; u = 1-4; v = 0-2. Methods of prepn. are claimed, comprising (a) reacting A-U-substituted oxirane or a protected form thereof in which a reactive substituent group is protected, with H2NCH2CH2VC6H4W-p or a protected form thereof in which a reactive substituent group is protected; and if required removing any protecting group to give 1. (b) reacting ACH(OPr)CH2I, wherein Pr is a protecting group, with H2NCH2CH2VC6H4W-p or a protected form thereof in which a reactive substituent group is protected; and if required removing any protecting group to give 1 wherein U represents a bond. (c) removing any protecting group from 1 in which at least one substituent carries a protecting group to give 1; or (d) converting a basic compd. 1 to a salt thereof by reaction with a pharmaceutically acceptable acid or (e) converting 1 having one or more reactive substituent groups to a different 1; or (f) isolating an isomer of 1 from a mixt. thereof. **391674-22-9P**, tert-Butyl 4-[2-(4-ethylphenyl)-3H-imidazo[4,5b]pyridin-3-yl]phenethylcarbamate 391674-24-1P, 2-[4-[2-(4-Ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]-1ethanamine formate 391674-25-2P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(4-ethylphenyl)-3Himidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol 391674-27-4P, tert-Butyl 4-(2-pentyl-3H-imidazo[4,5b]pyridin-3-yl)phenethylcarbamate 391674-28-5P, (2S) - 1 - [4 - [(tert-Butyldiphenylsilyl)oxy]phenoxy] - 3 - [[4 - (2-pentyl-3H-

IT

imidazo-[4,5-b]pyridin-3-yl)phenethyl]amino]-2-propanol **391674-34-3P**, tert-Butyl 4-[2-(2-cyclopentylethyl)-3Himidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-35-4P , 4-[2-(2-Cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3yl]phenethylamine 391674-36-5P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(2-cyclopentylethyl)-3Himidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol **391674-60-5P**, tert-Butyl 4-[2-[4-[[(hexylamino)carbonyl]amino]phenethyl]-3H-imidazo[4,5-b]pyridin-3yl]phenethylcarbamate 391674-63-8P, N-[4-[2-[3-[4-(2-Aminoethyl)phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]-N'hexylurea formate 391674-64-9P, N-[4-[2-[3-[4-[2-[[(2S)-3-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-2hydroxypropyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2yl]ethyl]phenyl]-N'-hexylurea (intermediate; prepn. of heterocyclic amino alc. beta-3 adrenergic receptor agonists) 391674-22-9 ZCA Carbamic acid, [2-[4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 391674-24-1 ZCA CN Formic acid, compd. with 4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]benzeneethanamine (9CI) (CA INDEX NAME)

CM 1

RN

CN

CRN 391674-23-0 CMF C22 H22 N4

CM 2

CRN 64-18-6 CMF C H2 O2

O = CH-OH

RN 391674-25-2 ZCA

CN 2-Propanol, 1-[4-[[(1,1-dimethylethyl)diphenylsilyl]oxy]phenoxy]-3-[[2-[4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3yl]phenyl]ethyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

__ Bu-t

RN 391674-27-4 ZCA

CN Carbamic acid, [2-[4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

RN 391674-28-5 ZCA

CN 2-Propanol, 1-[4-[[(1,1-dimethylethyl)diphenylsilyl]oxy]phenoxy]-3[[2-[4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl]amino]-,
(2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

___Bu-t

RN 391674-34-3 ZCA

CN Carbamic acid, [2-[4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$CH_2-CH_2$$
 $CH_2-CH_2-NH-C-OBu-t$
 $CH_2-CH_2-NH-C-OBu-t$

RN 391674-35-4 ZCA

CN Benzeneethanamine, 4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{CH}_2\text{--}\text{CH}_2 \\ \hline \\ N & \text{N} \\ \hline \\ \text{CH}_2\text{--}\text{CH}_2\text{--}\text{NH}_2 \\ \end{array}$$

RN 391674-36-5 ZCA

CN 2-Propanol, 1-[[2-[4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]-3-[4-[[(1,1-dimethylethyl)diphenylsilyl]oxy]phenoxy]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

__Bu-t

RN 391674-60-5 ZCA

CN Carbamic acid, [2-[4-[2-[4-[[(hexylamino)carbonyl]amino]phenyl]et hyl]-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ NH-C-NH-(CH_2)_5-Me \\ \hline \\ N-R \end{array}$$

RN 391674-63-8 ZCA

CN Formic acid, compd. with N-[4-[2-[3-[4-(2-aminoethyl)phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]-N'-hexylurea (9CI) (CA INDEX NAME)

CM 1

CRN 391674-62-7 CMF C29 H36 N6 O

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

CM 2

CRN 64-18-6 CMF C H2 O2

O = CH - OH

RN 391674-64-9 ZCA
CN Urea, N-[4-[2-[3-[4-[2-[[(2S)-3-[4-[[(1,1-dimethylethyl)diphenylsilyl]oxy]phenoxy]-2-hydroxypropyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]-N'-hexyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

__Bu-t

IT **391674-21-8P**, 4-[(2S)-3-[2-[4-[2-(4-Ethylphenyl)imidazo[4,5b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol hydrochloride 391674-26-3P, 4-[(2S)-2-Hydroxy-3-[2-[4-(2pentylimidazo[4,5-b]pyridin-3-yl)phenyl]ethylamino]propoxy]phenol **391674-33-2P**, 4-[(2S)-3-[2-[4-[2-(2-Cyclopentylethyl) imidazo[4,5-b] pyridin-3-yl] phenyl] ethylamino]-2hydroxypropoxy]phenol 391674-37-6P, 4-[3-[2-[4-[2-(2-Cyclopentylethyl) imidazo [4,5-b] pyridin-3-yl] phenyl] ethylamino] -2hydroxypropoxy]-1,3-dihydrobenzoimidazol-2-one monohydrochloride **391674-38-7P**, 4-[(2S)-2-Hydroxy-3-[2-[4-(2-pentylimidazo[4,5b]pyridin-3-yl)phenyl]ethylamino]propoxy]-1,3-dihydrobenzoimidazol-2one **391674-59-2P**, 1-Hexyl-3-[4-[2-[3-[4-[2-[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-3H-imidazo[4,5b]pyridin-2-yl]ethyl]phenyl]urea 391674-68-3P, 4-[3-[2-[4-[2-(2-Cyclopentylethyl)imidazo[4,5-b]pyridin-3yl]phenyl]ethylamino]-2-hydroxypropoxy]-1,3-dihydrobenzoimidazol-2one **391674-70-7P**, 4-[(2S)-3-[2-[4-[2-(4-Ethylphenyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2hydroxypropoxy] phenol

(prepn. of heterocyclic amino alc. beta-3 adrenergic receptor

agonists)

RN 391674-21-8 ZCA

CN Phenol, 4-[(2S)-3-[[2-[4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]-2-hydroxypropoxy]-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 391674-26-3 ZCA

CN Phenol, 4-[(2S)-2-hydroxy-3-[[2-[4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl]amino]propoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 391674-33-2 ZCA

CN Phenol, 4-[(2S)-3-[[2-[4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 391674-37-6 ZCA

CN 2H-Benzimidazol-2-one, 4-[3-[[2-[4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]-2-hydroxypropoxy]-1,3-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HN} \\ \text{O} \\ \text{H} \\ \text{CH}_2 \\ \text{HO-CH-CH}_2 - \text{NH-CH}_2 - \text{CH}_2 \\ \end{array}$$

● HCl

RN 391674-38-7 ZCA

CN 2H-Benzimidazol-2-one, 1,3-dihydro-4-[(2S)-2-hydroxy-3-[[2-[4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl]amino]propoxy]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 391674-59-2 ZCA

CN Urea, N-hexyl-N'-[4-[2-[3-[4-[2-[[(2S)-2-hydroxy-3-(4-hydroxyphenoxy)propyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-yl]ethyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & H & H \\ N & (CH_2)_{5} \end{array}$$
 Me
$$\begin{array}{c} N \\ N \\ N \end{array}$$
 OH

RN 391674-68-3 ZCA

CN 2H-Benzimidazol-2-one, 4-[3-[[2-[4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]-2-hydroxypropoxy]-1,3-dihydro-(9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{HN} \\ \text{O} \\ \text{H} \\ \text{CH}_2 \\ \text{HO-CH-CH}_2 - \text{NH-CH}_2 - \text{CH}_2 \\ \end{array}$$

RN 391674-70-7 ZCA

CN Phenol, 4-[(2S)-3-[[2-[4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]-2-hydroxypropoxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 391674-22-9P, tert-Butyl 4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-24-1P,
2-[4-[2-(4-Ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]-1-ethanamine formate 391674-25-2P, (2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(4-ethylphenyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol
391674-27-4P, tert-Butyl 4-(2-pentyl-3H-imidazo[4,5-b]pyridin-3-yl)phenethylcarbamate 391674-28-5P,
(2S)-1-[4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-(2-pentyl-3H-imidazo-[4,5-b]pyridin-3-yl)phenethyl]amino]-2-propanol
391674-34-3P, tert-Butyl 4-[2-(2-cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenethylcarbamate 391674-35-4P
, 4-[2-(2-Cyclopentylethyl)-3H-imidazo[4,5-b]pyridin-3-

```
yl]phenethylamine 391674-36-5P, (2S)-1-[4-[(tert-
     Butyldiphenylsilyl)oxy]phenoxy]-3-[[4-[2-(2-cyclopentylethyl)-3H-
     imidazo[4,5-b]pyridin-3-yl]phenethyl]amino]-2-propanol
     391674-60-5P, tert-Butyl 4-[2-[4-
     [[(hexylamino)carbonyl]amino]phenethyl]-3H-imidazo[4,5-b]pyridin-3-
     yl]phenethylcarbamate 391674-63-8P, N-[4-[2-[3-[4-(2-
     Aminoethyl) phenyl] -3H-imidazo[4,5-b] pyridin-2-yl] ethyl] phenyl] -N'-
     hexylurea formate 391674-64-9P, N-[4-[2-[3-[4-[2-[[(2S)-3-
     [4-[(tert-Butyldiphenylsilyl)oxy]phenoxy]-2-
     hydroxypropyl]amino]ethyl]phenyl]-3H-imidazo[4,5-b]pyridin-2-
     yl]ethyl]phenyl]-N'-hexylurea
         (intermediate; prepn. of heterocyclic amino alc. beta-3
        adrenergic receptor agonists)
     391674-21-8P, 4-[(2S)-3-[2-[4-[2-(4-Ethylphenyl)imidazo[4,5-
IT
     b]pyridin-3-yl]phenyl]ethylamino]-2-hydroxypropoxy]phenol
     hydrochloride 391674-26-3P, 4-[(2S)-2-Hydroxy-3-[2-[4-(2-
     pentylimidazo[4,5-b]pyridin-3-yl)phenyl]ethylamino]propoxy]phenol
     391674-33-2P, 4-[(2S)-3-[2-[4-[2-(2-
     Cyclopentylethyl) imidazo [4,5-b] pyridin-3-yl] phenyl] ethylamino] -2-
     hydroxypropoxy]phenol 391674-37-6P, 4-[3-[2-[4-[2-(2-
     Cyclopentylethyl) imidazo [4,5-b] pyridin-3-yl] phenyl] ethylamino] -2-
     hydroxypropoxy]-1,3-dihydrobenzoimidazol-2-one monohydrochloride
     391674-38-7P, 4-[(2S)-2-Hydroxy-3-[2-[4-(2-pentylimidazo[4,5-
     b]pyridin-3-yl)phenyl]ethylamino]propoxy]-1,3-dihydrobenzoimidazol-2-
     one 391674-59-2P, 1-Hexyl-3-[4-[2-[3-[4-[2-[(2S)-2-hydroxy-
     3-(4-hydroxyphenoxy)propylamino]ethyl]phenyl]-3H-imidazo[4,5-
     b]pyridin-2-yl]ethyl]phenyl]urea 391674-68-3P,
     4-[3-[2-[4-[2-(2-Cyclopentylethyl)imidazo[4,5-b]pyridin-3-
     yl]phenyl]ethylamino]-2-hydroxypropoxy]-1,3-dihydrobenzoimidazol-2-
     one 391674-70-7P, 4-[(2S)-3-[2-[4-[2-(4-
     Ethylphenyl)imidazo[4,5-b]pyridin-3-yl]phenyl]ethylamino]-2-
     hydroxypropoxy]phenol
         (prepn. of heterocyclic amino alc. beta-3 adrenergic receptor
        agonists)
     ANSWER 5 OF 13 ZCA COPYRIGHT 2003 ACS
L5
136:102370 Preparation of tetrahydropyridine or piperidine heterocyclic
     derivatives and their affinity for CRF receptors. Nakazato, Atsuro;
     Kumagai, Toshihito; Okubo, Taketoshi; Kameo, Kazuya (Taisho
     Pharmaceutical Co., Ltd., Japan). PCT Int. Appl. WO 2002002549 A1
     20020110, 91 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ,
     BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ,
     EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG,
     KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ,
     NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ,
     UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR.
     (English). CODEN: PIXXD2. APPLICATION: WO 2001-JP5806 20010704.
     PRIORITY: JP 2000-204021 20000705; JP 2000-270535 20000906.
AB
     Tetrahydropyridine or piperidine heterocyclic derivs. with high
     affinity for CRF receptors were prepd. E.g., 5-(4-carbamoyl-1,2,3,6-
```

tetrahydropyridin-1-yl)-2-(N-ethyl-2,4-dichloroanilino)-4-methylthiazole was prepd. by bromination of 2-(N-ethyl-2,4-dichloroanilino)-4-methylthiazole hydrochloride, followed by reaction with 5-carbamoyl-1,2,3,6-tetrahydropyridine hydrochloride. 388123-42-0P

(prepn. of tetrahydropyridine or piperidine heterocyclic derivs. and their affinity for CRF receptors)

RN 388123-42-0 ZCA

IT

CN 4-Pyridinecarboxamide, 1-[2-ethyl-5-methyl-3-(2,4,6-trimethylphenyl)-3H-imidazo[4,5-b]pyridin-7-yl]-1,2,3,6-tetrahydro-(9CI) (CA INDEX NAME)

IT 388123-42-0P

(prepn. of tetrahydropyridine or piperidine heterocyclic derivs. and their affinity for CRF receptors)

L5 ANSWER 6 OF 13 ZCA COPYRIGHT 2003 ACS

121:255405 Catechol diethers as selective phosphodiesterase IV
 inhibitors. Duplantier, Allen J.; Eggler, James F.; Marfat,
 Anthony; Masamune, Hiroko (Pfizer Inc., USA). PCT Int. Appl. WO
 9412461 A1 19940609, 159 pp. DESIGNATED STATES: W: AU, BR, CA, CZ,
 JP, KR, NO, NZ, PL, RU, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR,
 IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2.
 APPLICATION: WO 1993-US10228 19931029. PRIORITY: US 1992-984408
 19921202.

The title compds. [I; A, B = direct bond, (un) substituted C1-5 AB alkylene, (un) substituted alkenyl, (un) substituted phenylene; R1 = Me, Et, CF2H, CF3; R2 = C1-6 alkyl, alkoxyalkyl, phenoxyalkyl, cycloalkyl, etc.; Y = direct bond, O, NR6, S; R6 = H, C1-4 alkyl; Z = (un) substituted monocyclic or bicyclic heterocyclyl], which are inhibitors of phosphodiesterase IV (no data), useful in the treatment of inflammatory conditions (no data), etc., are prepd. Thus, 3-(carbomethoxy) benzyltriphenylphosphonium bromide was reacted with 3-cyclopentyloxy-4-methoxybenzaldehyde in the presence of BuLi, producing Me 3-[2-[3-(cyclopentyloxy)-4-

methoxyphenyl]ethenyl]benzoate (36% cis-isomer, 36% trans-isomer).

158427-58-8P IT

(prepn. and phosphodiesterase IV inhibitory activity of)

RN 158427-58-8 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 3-[4-[[3-(bicyclo[2.2.1]hept-2-yloxy)-4methoxyphenyl]methoxy]phenyl]-2-butyl-, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 158429-25-5P

> (prepn. and reaction of, in prepn. of catechol diether phosphodiesterase IV inhibitors)

158429-25-5 ZCA RN

Phenol, 4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)- (9CI) (CA INDEX CN NAME)

IT 158429-25-5

(reaction of, in prepn. of catechol diether phosphodiesterase IV inhibitors)

RN 158429-25-5 ZCA

CN Phenol, 4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)- (9CI) (CA INDEX NAME)

IT 158427-58-8P

(prepn. and phosphodiesterase IV inhibitory activity of)

IT 158429-25-5P

(prepn. and reaction of, in prepn. of catechol diether phosphodiesterase IV inhibitors)

IT 158429-25-5

(reaction of, in prepn. of catechol diether phosphodiesterase IV inhibitors)

L5 ANSWER 7 OF 13 ZCA COPYRIGHT 2003 ACS

121:222008 Heterocyclic angiotensin II receptor antagonists for therapeutic use. Carpino, Philip C.; Wester, Ronald T.; Jardine, Paul A. Da Silva (Pfizer Inc., USA). U.S. US 5338740 A 19940816, 21 pp. (English). CODEN: USXXAM. APPLICATION: US 1993-91099 19930713.

Heterocyclic compds. Ar-W-Het [Ar = thienyl, 6-membered N-contg. heterocycle; W = carbobicyclic or heterobicyclic spacer group; Het = (substituted) imidazolyl, 1,3-diazaspiro[4.4]nonenyl, imidazo[4,5-b]pyridyl, quinazolinyl] are regulators of the action of angiotensin II in mammals, useful in the treatment and prevention of hypertension, glaucoma, renal disease, congestive heart failure, cognitive dysfunction, and other conditions in which the action of angiotensin II is implicated. These compds. were effective against exptl. hypertension in rats at 0.1-30 mg/kg orally or 0.01-10 mg/kg parenterally. Thus, 2-butyl-5-chloro-1-[5-[2-(1H-tetrazol-5-yl)phenyl]indan-1-yl]-1H-imidazole-4-carboxylic acid was prepd. in 7 steps from 5-bromoindan-1-one, 2-bromobenzonitrile, and 2-butyl-5-chloro-1H-imidazol-4-ylmethanol.

IT 154122-29-9 154122-31-3 158330-80-4

158330-85-9 158330-86-0

(heterocyclic angiotensin II receptor antagonists for therapeutic use)

RN 154122-29-9 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[1,2,3,4-tetrahydro-6-[2-(1H-tetrazol-5-yl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 154122-31-3 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[6-[2-(1H-tetrazol-5-yl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 158330-80-4 ZCA

CN Benzoic acid, 2-[5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-5,6,7,8-tetrahydro-2-naphthalenyl]- (9CI) (CA INDEX NAME)

RN

158330-85-9 ZCA Benzoic acid, 2-[5-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)-2-CNnaphthalenyl] - (9CI) (CA INDEX NAME)

RN 158330-86-0

3H-Imidazo[4,5-b]pyridine, 2-butyl-3-[6-[2-(1H-tetrazol-5-yl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME) CN

IT 154122-52-8P 154122-53-9P 158331-08-9P 158331-09-0P 158331-10-3P 158331-11-4P 158331-17-0P 158331-26-1P 158331-27-2P 158331-28-3P 158331-29-4P 158331-30-7P 158331-31-8P 158331-33-0P

(heterocyclic angiotensin II receptor antagonists for therapeutic use)

RN 154122-52-8 ZCA

CN 2-Naphthalenol, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)- (9CI) (CA INDEX NAME)

RN 154122-53-9 ZCA

CN Methanesulfonic acid, trifluoro-, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)

Me N Et O
$$\sim$$
 CF3

RN 158331-08-9 ZCA

CN 2-Naphthalenol, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-5,6,7,8-tetrahydro-(9CI) (CA INDEX NAME)

RN 158331-09-0 ZCA

CN Methanesulfonic acid, trifluoro-, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-5,6,7,8-tetrahydro-2-naphthalenyl ester (9CI) (CA INDEX NAME)

RN 158331-10-3 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[1,2,3,4-tetrahydro-6-(tributylstannyl)-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 158331-11-4 ZCA

CN Benzoic acid, 2-[5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-5,6,7,8-tetrahydro-2-naphthalenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 158331-17-0 ZCA

CN 2-Naphthaleneacetonitrile, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-5,6,7,8-tetrahydro-.alpha.-oxo- (9CI) (CA INDEX NAME)

RN 158331-26-1 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-butyl-3-[6-(phenylmethoxy)-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 158331-27-2 ZCA

CN 2-Naphthalenol, 5-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)- (9CI) (CA INDEX NAME)

RN 158331-28-3 ZCA

CN Methanesulfonic acid, trifluoro-, 5-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
N & Bu-n \\
\hline
0 & \\
0 - S - CF_3 \\
\hline
0
\end{array}$$

RN 158331-29-4 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-butyl-3-[6-(tributylstannyl)-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 158331-30-7 ZCA

CN Benzoic acid, 2-[5-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)-2-naphthalenyl]-, methyl ester (9CI) (CA INDEX NAME)

RN 158331-31-8 ZCA

CN Benzonitrile, 2-[5-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)-2-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 158331-33-0 ZCA CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[6-[2-[1-(triphenylmethyl)-1H-tetrazol-5-yl]phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

IT 154122-29-9 154122-31-3 158330-80-4

158330-85-9 158330-86-0

(heterocyclic angiotensin II receptor antagonists for therapeutic use)

IT 154122-52-8P 154122-53-9P 158331-08-9P

158331-09-0P 158331-10-3P 158331-11-4P

158331-17-0P 158331-26-1P 158331-27-2P

158331-28-3P 158331-29-4P 158331-30-7P

158331-31-8P 158331-33-0P

(heterocyclic angiotensin II receptor antagonists for therapeutic use)

L5 ANSWER 8 OF 13 ZCA COPYRIGHT 2003 ACS

121:458 Dihydropyridines: a new class of angiotensin II antagonists.
Wester, Ronald T.; Jularski, Christian J.; Magnus-Ayritey, George
T.; da Silva Jardine, Paul; LaFlamme, Janet S.; Berke, Helen;
Bussolotti, Donald L.; Rauch, Albert L.; Hoover, Karen W. (Dep. Med. Chem., Pfizer Cent. Res., Groton, CT, 06340, USA). Bioorganic &
Medicinal Chemistry Letters, 4(1), 133-8 (English) 1994. CODEN:

BMCLE8. ISSN: 0960-894X.

GI

AB The synthesis and biol. activities of dihydropyridine angiotensin II (AII) antagonists are described. Compds. such as I are examples of a new, structurally distinct class for AT1-selective agents.

IT 154668-33-4 154668-35-6

(angiotensin II antagonists activity of)

RN 154668-33-4 ZCA

CN 3-Pyridinecarboxylic acid, 4-(2-chlorophenyl)-1,4-dihydro-2,6-dimethyl-5-[(2-pyridinylamino)carbonyl]-, 2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

RN 154668-35-6 ZCA

CN 3-Pyridinecarboxylic acid, 4-(2-chlorophenyl)-1,4-dihydro-6-methyl-2-(1-methylethyl)-5-[(2-pyridinylamino)carbonyl]-,
2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester (9CI)
(CA INDEX NAME)

IT 154668-32-3P

(prepn. and Hantzsch reaction of, with enamine deriv.)

RN 154668-32-3 ZCA

CN Butanoic acid, 2-[(2-chlorophenyl)methylene]-3-oxo-,

2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

IT 154668-37-8P 154668-45-8P

(prepn. and angiotensin II antagonists activity of)

RN 154668-37-8 ZCA

CN 3-Pyridinecarboxylic acid, 4-(2-chlorophenyl)-1,4-dihydro-6-methyl-2-(1-methylethyl)-5-[(3-pyridinylamino)carbonyl]-,

2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester, (-)-(9CI) (CA INDEX NAME)

Rotation (-).

RN 154668-45-8 ZCA

CN 3-Pyridinecarboxylic acid, 4-(2-chlorophenyl)-1,4-dihydro-6-methyl-2-(1-methylethyl)-5-[(3-pyridinylamino)carbonyl]-,
2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester, (+)-(9CI) (CA INDEX NAME)

Rotation (+).

IT 154668-36-7P

(prepn. and condensation with chlorobenzaldehydes)

RN 154668-36-7 ZCA

CN Pentanoic acid, 4-methyl-3-oxo-, 2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

IT 154668-31-2P

(prepn. and reaction with chlorobenzaldehyde)

RN 154668-31-2 ZCA

CN Butanoic acid, 3-oxo-, 2-[4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl ester (9CI) (CA INDEX NAME)

IT 154668-34-5P

(prepn. and reaction with diketene)

RN 154668-34-5 ZCA

CN Benzeneethanol, 4-(2-butyl-3H-imidazo[4,5-b]pyridin-3-yl)- (9CI) (CA INDEX NAME)

IT 154668-33-4 154668-35-6

(angiotensin II antagonists activity of)

IT 154668-32-3P

(prepn. and Hantzsch reaction of, with enamine deriv.)

IT 154668-37-8P 154668-45-8P

(prepn. and angiotensin II antagonists activity of)

IT 154668-36-7P

(prepn. and condensation with chlorobenzaldehydes)

IT 154668-31-2P

(prepn. and reaction with chlorobenzaldehyde)

IT 154668-34-5P

(prepn. and reaction with diketene)

L5 ANSWER 9 OF 13 ZCA COPYRIGHT 2003 ACS

120:235407 A conformationally restrained series of AT1-selective angiotensin II antagonists. Carpino, Philip A.; Sneddon, Scott F.; da Silva Jareine, Paul; Magnus-Ayritey, George T.; Rauch, Albert L.; Burkard, Michael R. (Dep. Med. Chem., Pfizer Cent. Res., Croton, CT, 06340, USA). Bioorganic & Medicinal Chemistry Letters, 4(1), 93-8 (English) 1994. CODEN: BMCLE8. ISSN: 0960-894X.

GI

IT

AB The benzyl linker in the angiotensin II receptor antagonist L-158,809 (I) that separates the imidazo[4,5-b]pyridine ring and the 2-tetrazolylphenyl groups was replaced by a series of bicyclic rings. The optimal bicyclic ring was found to be a dihydroindanyl group. Modification of the imidazo[4,5-b]pyridine group resulted in the discovery of a rigid analog that was potent as L-158,809.

154122-29-9P 154122-31-3P (prepn. and angiotensin II antagonist activity of, conformationally restrained)

RN 154122-29-9 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[1,2,3,4-tetrahydro-6-[2-(1H-tetrazol-5-yl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

RN 154122-31-3 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[6-[2-(1H-tetrazol-5-yl)phenyl]-1-naphthalenyl]- (9CI) (CA INDEX NAME)

IT 154122-53-9P

(prepn. and cross coupling of, with trityltetrazolylboronic acid and tetrakis(triphenylphosphine)palladium)

RN 154122-53-9 ZCA

CN Methanesulfonic acid, trifluoro-, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-2-naphthalenyl ester (9CI) (CA INDEX NAME)

Me N Et O
$$S-CF_3$$

IT 154122-47-1P

(prepn. and reaction of, with trimethyltin azide)

RN 154122-47-1 ZCA

CN Benzonitrile, 2-[5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)-5,6,7,8-tetrahydro-2-naphthalenyl]- (9CI) (CA INDEX NAME)

IT 154122-52-8P

(prepn. and triflation of)

RN 154122-52-8 ZCA

CN 2-Naphthalenol, 5-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)- (9CI) (CA INDEX NAME)

IT 154122-29-9P 154122-31-3P

(prepn. and angiotensin II antagonist activity of, conformationally restrained)

IT 154122-53-9P

(prepn. and cross coupling of, with trityltetrazolylboronic acid and tetrakis(triphenylphosphine)palladium)

IT 154122-47-1P

(prepn. and reaction of, with trimethyltin azide)

IT 154122-52-8P

(prepn. and triflation of)

L5 ANSWER 10 OF 13 ZCA COPYRIGHT 2003 ACS 115:135998 Potent, orally active imidazo[4,5-b]pyridine-based

angiotensin II receptor antagonists. Mantlo, Nathan B.; Chakravarty, Prasun K.; Ondeyka, Debra L.; Siegl, Peter K. S.; Chang, Raymond S.; Lotti, Victor J.; Faust, Kristie A.; Schorn, Terry W.; Chen, Tsing Bau; et al. (Explor. Chem., Merck Sharp and Dohme Res. Lab., Rahway, NJ, 07065, USA). Journal of Medicinal Chemistry, 34(9), 2919-22 (English) 1991. CODEN: JMCMAR. ISSN:

0022-2623.

GI

AB Several title Angiotensin II (AII) antagonists I (R = Et, Pr, Bu, R1

= R2 = H, Me; R1 = Me, R2 = H; R1 = H, R2 = Me) were prepd. Substituents at the 2, 5, and 7-positions of the imidazopyridine have a profound effect on the in vitro binding affinity to AII receptors (rabbit aorta membrane prepn.) and on the inhibition of the AII-induced pressor responses in conscious rats. The most active compd., I (R = Et, R1 = R2 = Me) is extremely potent in vitro (IC50 = 0.3 nM, rabbit aorta), and in vivo (ED50 = 0.048 mg/Kg i.v. and 0.026 mg/Kg p.o., conscious rat). This compd. is a specific AT1 antagonist, and substantially lowers the blood pressure of high renin hypertensive rats upon oral dosing (0.1 and 0.3 mg/Kg) with a duration of action exceeding 24 h.

IT 135145-91-4P 135145-92-5P 135145-93-6P 135145-94-7P 135145-95-8P 135145-96-9P

(prepn. and Angiotensin II antagonist activity of)

RN 135145-91-4 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-propyl-3-[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

RN 135145-92-5 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 5-methyl-2-propyl-3-[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

RN 135145-93-6 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 7-methyl-2-propyl-3-[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

RN 135145-94-7 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-butyl-5,7-dimethyl-3-[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

RN 135145-95-8 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 5,7-dimethyl-2-propyl-3-[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

RN 135145-96-9 ZCA

CN 3H-Imidazo[4,5-b]pyridine, 2-ethyl-5,7-dimethyl-3-[2'-(1H-tetrazol-5-yl)[1,1'-biphenyl]-4-yl]- (9CI) (CA INDEX NAME)

IT 135145-91-4P 135145-92-5P 135145-93-6P 135145-94-7P 135145-95-8P 135145-96-9P (prepn. and Angiotensin II antagonist activity of)

L5 ANSWER 11 OF 13 ZCA COPYRIGHT 2003 ACS 84:43936 2-Aldehydes of imidazo[4,5-b] - and imidazo[4,5-c]pyridines. Yutilov, Yu. M.; Kovaleva, L. I. (Donetsk. Otd. Fiz.-Org. Khim., Inst. Fiz. Khim. im. Pisarzhevskogo, Donetsk, USSR). Khimiya Geterotsiklicheskikh Soedinenii (10), 1389-93 (Russian) 1975. CODEN: KGSSAQ. ISSN: 0132-6244.

GI For diagram(s), see printed CA Issue.

Imidazopyridinecarboxaldehydes (I, R = Me, PhCH2, Ph, R1 = CHO), II (R1 = CHO), III (R1 = CHO), and IV (R = PhCH2, Ph, R1 = CHO) were obtained in 50-84% yields by oxidn. of the corresponding 2-methyl deriv. with SeO2 in dioxane at 70-80.degree.. Condensation of the aldehydes with CH2(CO2H)2 gave 43-60% acrylic acid derivs. I (R = Me, R1 = CH:CHCO2H). II (R1 = CH:CHCO2H), and IV (R = Ph, R1 = CH:CHCO2H). The cyano derivs. I (R = Me, PhCH2R1 = CN), II (R1 = CN), and IV (R = PhCH2, Ph, R1 = CN) were obtained in 65-93% by boiling the corresponding aldoximes with Ac2O 7 hr. Amides I (R = Me, PhCH2, R1 = CONM2), II (R1 = CONH2), and IV (R = Ph, R1 = CONH2) were obtained in 60-82% yields by oxidn. of the corresponding nitriles with concd. H2SO4.

IT 57806-16-3P

(prepn. of)

RN 57806-16-3 ZCA

CN 2-Propenoic acid, 3-(3-phenyl-3H-imidazo[4,5-b]pyridin-2-yl)- (9CI) (CA INDEX NAME)

IT **57806-16-3P** (prepn. of)

L5 ANSWER 12 OF 13 ZCA COPYRIGHT 2003 ACS

78:159570 Reactions of .beta.-keto esters with 2,3-diaminopyridine and its derivatives. Israel, Mervyn; Jones, Lynne C. (Child. Cancer Res. Found, Boston, MA, USA). Journal of Heterocyclic Chemistry, 10(2), 201-7 (English) 1973. CODEN: JHTCAD. ISSN: 0022-152X.

AB Results from diamine-ketoester condensations were compared in an attempt to develop generalizations of predictive value regarding the direction of ring closure to form diazepinones. Condensation reactions described are: 2,3-diaminopyridine with 2-(ethoxycarbonyl)cyclohexanone and with Et .alpha.-methylacetoacetate, 5-bromo-2,3-diamino-4-methyllpyridine with AcCH2CO2Et (I), 3-amino-2-anilinopyridine and 3-amino-2-(methylamino)pyridine with I, and N-methyl-.omicron.-phenylenediamine with I.

IT 41231-00-9P

(prepn. of)

RN 41231-00-9 ZCA

CN 2-Propanone, 1-(3-phenyl-3H-imidazo[4,5-b]pyridin-2-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \circ & \circ \\ & | \\ & | \\ & \mathsf{CH_2} - \mathsf{C-Me} \end{array}$$

IT **41231-00-9P** (prepn. of)

L5 ANSWER 13 OF 13 ZCA COPYRIGHT 2003 ACS
64:68496 Original Reference No. 64:12858e-h,12859a-c
1H-Imidazo[4,5-b]quinocarbocyanine iodides. Jenkins, Philip W.; S.
Brooker, Leslie G. (Kodak-Pathe). FR 1400756 19650528, 12 pp.
(Unavailable). PRIORITY: US 19630610.

GI For diagram(s), see printed CA Issue.

The title compds. are prepd. and can be used to sensitize Ag AB bromoiodide (I) and Ag chlorobromide (II) emulsions. Thus, a mixt. of 3.6 q. 2,3-dimethyl-4-oxo-1-phenyl-2-imidazolinium p-toluenesulfonate, 1.2 g. o-H2NC6H4CHO, and 15 ml. HOAc is refluxed for 2.2 hrs. to give III (R = R1 = Me, R2 = Ph, X = p-MeC6H4SO3) Similar III prepd. are (R, R1, R2, X, and m.p. given): Et, Me, Ph, iodine (V) 230.5-2.5.degree. (EtOH); Et, Me, Et, iodine (VI), 186.0-7.5.degree. (EtOH). A mixt. of 30 ml. BuOH, 6.6 g. V and 12.0 g. PhN: CHOEt is refluxed 30 min. to give 75% III (R = Et, R1 = PhNHCH:CH, R2 = Ph, X = iodine, m. 263.0-4.0.degree. (decompn.) (MeOH). A mixt. of 10 ml. pyridine, 4.5 g. IV, 6.5 g. (EtO) 2CHOAc, and 1.0 g. Et3N is refluxed 10 min. and treated with a soln. of 4 g. KI in 50 ml. H2O to give 3% 3,3'-dimethyl-1,1'-diphenyl-IHimidazo[4,5-b]quinocarbocyanine iodide, m. 277.5-8.5.degree.

(decompn.) (MeOH), sensitization range (in a I emulsion) 520-665 m.mu., .lambda.max. 600 m.mu.. Similarly prepd. are the following VI [n, m.p., sensitization range in m.mu. (emulsion), and .lambda.max. in m.mu. given]: 0, 302.5-3.5.degree. (MeOH), .ltoreq.680 (I), 630; 1, 264.5-6.5.degree. (MeOH), 620-760 (I), 710; 2, 263.5-4.5.degree. (decompn.) (cresol-MeOH), --, --. A mixt. of 10 ml. EtOH, 0.9 g. VI, 1.1 g. 2-(.beta.-acetanilidovinyl)-3ethylbenzoxazolium iodide, and 0.25 mg. Et3N is refluxed to 20 min. to give 8% 1,3,3'-triethyl-1H-imidazo[4,5-b] quinooxacarbocyanine iodide, m. 245.0-6.0.degree. (decompn.) (MeOH), sensitization range (in a I emulsion) .ltoreq.615 m.mu., .lambda.max. 550 m.mu.. Similarly prepd. are the following VIII (R, R', m.p., sensitization range in m.mu. [emulsion], and .lambda.max. in m.mu. given): N-ethylbenzothiazolidin-2-ylidene-methyl, Et, 251-2.degree. (MeOH), .ltoreq.670 [I], 590 and 630; N-ethyl-1,2-dihydroquinolin-2ylidenemethyl, Et, 265.5-6.5.degree. (decompn.) (MeOH), .ltoreq.720 [I], 580 and 670; 1,3,3-trimethylindolin-2-ylidenemethyl, Ph, 312.5-13.5.degree. (decompn.) (MeOH), 510-625 [I], 590; p-Me2NC6H4, Ph, 288.5-9.5.degree. (decompn.) (MeOH), .ltoreq.630 [I], 585; p-Me2NC6H4CH:CH, Ph, 261.5-2.5.degree. (decompn.) (MeOH), .ltoreq.630 [I], 585. Also prepd. is 1-ethyl-5-[(3-ethyl-1-phenyl-1H-imidazo[4,5-b]quinol-2(3H)-ylidene)ethylidenel-2-thiobarbituric acid, >310.degree. (MeOH), .ltoreq.580 [II], .lambda.max. 540 m.mu.. Also prepd. are IX (R, R', n, X, Y, m.p. sensitization range in m.mu. [emulsion] and .lambda.max. in m.mu. given): Et, Et, O, O, S, 258-9.degree. (decompn.) (pyridine-MeOH), .ltoreg.630 [I], 570; Et, Et, 0, S, S, 249-50.degree. (decompn.) (pyridine-MeOH), .ltoreq.680 [I], 610; Ph, Et, 0, NPh, S, 225.5-6.5.degree. (decompn.) (pyridine-MeOH), .ltoreq.640 [II], 556 and 585; Ph, Ph, O, S, O, >300.degree. (pyridine-MeOH), 490-630 [II], 590; Ph, CH2CO2H, 0, O, S, 247.0-9.0.degree. (decompn.) (MeOH), .ltoreq.600 [I], 520 and 570; Ph, CH2CH2SO3H, 0, 0, S, 291.5-2.5.degree. (decompn.), .ltoreq.635 [I], 570; Ph, Et, 1, S, S, 235.5-6.5.degree. (decompn.) (ligroine), 560-750 [II], 700. 102032-37-1, Barbituric acid, 1-ethyl-5-[2-(1-ethyl-1,3dihydro-3-phenyl-2H-imidazo-[4,5-b]quinolin-2-ylidene)ethylidene]-2thio- 102344-95-6, 2,4-Thiazolidinedione, 5-[2-(3-ethyl-1-phenyl-1H-imidazo[4,5-b]quinolin-2(3H)ylidene)ethylidene]-3-phenyl-(prepn. of) 102032-37-1 ZCA

RN 102032-37-1 ZCA CN Barbituric acid, 1-ethyl-5-[2-(1-ethyl-1,3-dihydro-3-phenyl-2H-imidazo-[4,5-b]quinolin-2-ylidene)ethylidene]-2-thio-(7CI) (CAINDEX NAME)

IT

RN 102344-95-6 ZCA CN 2,4-Thiazolidinedione, 5-[2-(3-ethyl-1-phenyl-1H-imidazo[4,5-b]quinolin-2(3H)-ylidene)ethylidene]-3-phenyl- (7CI) (CA INDEX NAME)

IT 102032-37-1, Barbituric acid, 1-ethyl-5-[2-(1-ethyl-1,3-dihydro-3-phenyl-2H-imidazo-[4,5-b]quinolin-2-ylidene)ethylidene]-2-thio- 102344-95-6, 2,4-Thiazolidinedione, 5-[2-(3-ethyl-1-phenyl-1H-imidazo[4,5-b]quinolin-2(3H)-ylidene)ethylidene]-3-phenyl-(prepn. of)

=> d 15 2,3 cbib abs fhitstr hitrn

ZCA COPYRIGHT 2003 ACS L5 ANSWER 2 OF 13 136:340677 Preparation of imidazoarenes as antiinflammatory and analgesic agents.. Nakao, Kazunari; Okumura, Yoshiyuki; Matsumizu, Miyako; Uneo, Naomi; Hashizume, Yoshinobu; Kato, Tomoki; Kawai, Akiyoshi; Miyake, Yoriko; Nukui, Seiji; Shinjyo, Katsuhiro; Taniquchi, Kana (Pfizer Pharmaceuticals Inc., Japan; Pfizer Inc.). PCT Int. Appl. WO 2002032900 A2 20020425, 461 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ; TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). APPLICATION: WO 2001-IB1940 20011015. PRIORITY: US

2000-PV241825 20001019.

GI

Title compds. [I; Y1-Y4 = N, CH, CL; R1 = H, (substituted) alkyl, AB alkenyl, alkynyl, cycloalkyl, alkoxy, pyrrolidinyl, amino, etc.; A = (substituted) 5-6 membered monocyclic arom. ring optionally contg. up to 3 heteroatoms selected from O, N, S, etc.; B = halo-substituted alkylene, cycloalklylene, alkenylene, alkynylene, alkyleneoxy, etc., optionally substituted with an oxo group; W = amino, O, S, bond, etc.; R2 = H, OH, alkyl, alkoxy; Z = 5-12 membered (substituted) monocyclic or bicyclic aryl optionally contg. up to 3 heteroatoms selected from O, N and S, etc.; L = halo, alkyl, haloalkyl, OH, alkoxy, haloalkoxy, alkylthio, NO2, amino, etc.], were prepd. as prostaglandin E2 receptor antagonists, preferably as EP4 receptor antagonists. Thus, to 2-[4-(2-ethyl-5,7-dimethyl-3Himidazo[4,5-b]pyridin-3-yl)phenyl]ethylamine (prepn. given) in CH2Cl2 was added p-toluenesulfonyl isocyanate followed by stirring for 3 h to give 56% 2-ethyl-5,7-dimethyl-3-[4-[2-[[[(4methylphenyl) sulfonyl] amino] carbonyl] amino] ethyl] phenyl] -3Himidazo[4,5-b]pyridine. Preferred I inhibited PGE2-induced thermal hyperalgesia in rats with ED50<60 mg/kg.

IT 415903-03-6P

(prepn. of imidazoarene prostaglandin EP4 receptor antagonists as antiinflammatory and analgesic agents)

RN 415903-03-6 ZCA

CN Benzenesulfonamide, N-[[[2-[4-[5,7-dimethyl-2-(1-methylethyl)-3H-imidazo[4,5-b]pyridin-3-yl]phenyl]ethyl]amino]carbonyl]-4-methyl-(9CI) (CA INDEX NAME)

IT 415903-03-6P 415903-06-9P 415903-08-1P 415903-10-5P 415903-29-6P

(prepn. of imidazoarene prostaglandin EP4 receptor antagonists as

```
antiinflammatory and analgesic agents)
IT
     415902-96-4P 415902-97-5P 415902-98-6P
     415902-99-7P 415903-00-3P 415903-01-4P
     415903-02-5P 415903-05-8P 415903-07-0P
     415903-09-2P 415903-11-6P 415903-12-7P
     415903-13-8P 415903-14-9P 415903-15-0P
     415903-16-1P 415903-17-2P 415903-18-3P
    415903-19-4P 415903-20-7P 415903-22-9P
    415903-24-1P 415903-26-3P 415903-28-5P
     415903-30-9P 415903-31-0P 415903-32-1P
    415903-33-2P 415903-34-3P 415903-35-4P
    415903-36-5P 415904-25-5P 415904-26-6P
    415904-27-7P 415904-28-8P 415904-29-9P
     415904-30-2P 415904-31-3P 415904-32-4P
    415904-33-5P 415904-34-6P 415904-35-7P
    415904-36-8P 415904-37-9P 415904-39-1P
    415904-40-4P 415904-41-5P 415904-42-6P
    415904-43-7P 415904-44-8P 415904-45-9P
    415904-46-0P 415904-47-1P 415904-48-2P
    415904-49-3P 415904-50-6P 415904-51-7P
    415904-52-8P 415904-53-9P 415904-54-0P
    415904-55-1P 415904-56-2P 415904-57-3P
    415904-58-4P 415904-59-5P 415904-60-8P
    415904-61-9P 415904-62-0P 415904-63-1P
    415904-64-2P 415904-65-3P 415904-66-4P
    415904-67-5P 415904-68-6P 415904-69-7P
    415904-72-2P 415904-76-6P 415904-77-7P
    415904-78-8P 415904-79-9P 415904-80-2P
    415904-86-8P 415904-88-0P 415904-90-4P
    415904-94-8P 415905-00-9P 415905-04-3P
    415905-08-7P 415905-11-2P 415905-13-4P
    415905-17-8P 415905-19-0P 415905-23-6P
    415905-25-8P 415905-27-0P 415905-33-8P
    415905-35-0P 415905-37-2P 415905-40-7P
    415905-42-9P 415905-49-6P 415905-51-0P
    415905-53-2P 415905-55-4P 415905-57-6P
    415905-59-8P 415905-63-4P 415905-69-0P
    415905-71-4P 415905-73-6P 415905-75-8P
    415905-77-0P 415905-80-5P 415906-11-5P
    415906-28-4P 415906-29-5P 415906-30-8P
    415906-31-9P 415906-38-6P 415906-39-7P
    415906-40-0P 415906-41-1P 415906-46-6P
    415906-47-7P 415906-48-8P 415906-50-2P
    416844-61-6P 416844-62-7P 416844-63-8P
    416844-69-4P 416844-70-7P 416844-71-8P
    416844-72-9P 416844-73-0P 416844-74-1P
     416844-75-2P
        (prepn. of imidazoarene prostaglandin EP4 receptor antagonists as
        antiinflammatory and analgesic agents)
IT
    415902-95-3P 415903-21-8P 415903-23-0P
     415903-25-2P 415903-27-4P 415906-27-3P
     415907-59-4P 415907-60-7P 415907-61-8P
```

```
415907-62-9P 415907-63-0P 415907-64-1P
415907-67-4P 415907-68-5P 415907-69-6P
415907-70-9P 415907-72-1P 415907-74-3P
415907-75-4P 415907-76-5P 415907-77-6P
415907-78-7P 415907-82-3P 415907-83-4P
415907-84-5P 415907-85-6P 415907-86-7P
415907-87-8P 415907-88-9P 415907-89-0P
415907-90-3P 415907-91-4P 415907-92-5P
415907-93-6P 415907-94-7P 415907-95-8P
415907-96-9P 415907-97-0P 415907-98-1P
415907-99-2P 415908-00-8P 415908-01-9P
415908-04-2P 415908-05-3P 415908-06-4P
415908-07-5P 415908-10-0P 415908-11-1P
415908-12-2P 415908-13-3P 415908-16-6P
415908-17-7P 415908-18-8P 415908-19-9P
415908-22-4P 415908-23-5P 415908-24-6P
415908-25-7P 415908-28-0P 415908-29-1P
415908-30-4P 415908-31-5P 415908-35-9P
415908-36-0P 415908-38-2P 415908-39-3P
415908-41-7P 415908-47-3P 415908-49-5P
415908-51-9P 415908-53-1P 415908-55-3P
415908-59-7P 415908-60-0P 415908-62-2P
415908-64-4P 415908-65-5P 415908-68-8P
415908-69-9P 415908-70-2P 415908-71-3P
415908-72-4P 415908-75-7P 415908-76-8P
415908-77-9P 415908-78-0P 415908-79-1P
415908-80-4P 415908-81-5P 415908-86-0P
415908-87-1P 415908-88-2P 415908-89-3P
415912-18-4P 415912-19-5P 415912-22-0P
415912-23-1P 415912-26-4P 415912-27-5P
415912-39-9P 415912-40-2P 415912-41-3P
415912-42-4P 415912-43-5P 415912-46-8P
415912-47-9P 415912-48-0P 415912-49-1P
415912-50-4P 415912-57-1P 415912-58-2P
415912-59-3P 415912-60-6P 415912-61-7P
415912-65-1P 415912-66-2P 415912-67-3P
415912-68-4P 415912-69-5P 415912-84-4P
415914-74-8P
```

(prepn. of imidazoarene prostaglandin EP4 receptor antagonists as antiinflammatory and analgesic agents)

ANSWER 3 OF 13 ZCA COPYRIGHT 2003 ACS L5136:340676 Preparation of benzimidazole derivatives as prostaglandin EP4 receptor inhibitors to treat rheumatoid arthritis. Audoly, Laurent; Okumura, Takako; Shimojo, Masato (Pfizer Pharmaceuticals Inc., Japan; Pfizer Inc.). PCT Int. Appl. WO 2002032422 A2 20020425, 468 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO,

NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM;

RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2001-IB1942 20011015. PRIORITY: US 2000-PV241825 20001019.

GI

AΒ Benzimidazole derivs. I wherein Y1-Y4 are independently N, CH, alkyl, alkoxy, haloalkyl, halo, substituted alkyl, R1 is H, alkyl, alkenyl, alkynyl, cycloalkyl, alkoxy, haloalkoxy, heterocycle; R2 is H, alkyl, alkoxy, OH; A is substituted heterocycle arom ring; B is haloalkylene, cycloalkylene, alkenylene, alkynylene, oxyalkylene; W is NH, aminoalkyl, O, S, oxime, covalent bond; Z is monocyclic and bicyclic arom. heterocycle, were prepd. as prostaglandin EP4 receptor inhibitors to treat rheumatoid arthritis of rats and human. Also featured is a method of identifying agents that selectively inhibit EP4 activity in vivo. Thus, $3-(4-\{2[(\{[(3,4$ dichlorophenyl) sulfonyl] amino { carbonyl) amino] ethyl } phenyl) -2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridine, hydrochloride was prepd. and tested in vivo as an agent selectively inhibiting EP4 activity or selectively binding EP4; and measuring joint inflammation, joint swelling, joint ankylosis, interleukin (IL)-6, SAA protein, and/or joint mobility.

IT 415902-96-4P

(prepn. of benzimidazole derivs. as prostaglandin ep receptor inhibitors to treat rheumatoid arthritis)

RN 415902-96-4 ZCA

CN Benzenesulfonamide, N-[[[2-[4-(2-ethyl-5,7-dimethyl-3H-imidazo[4,5-b]pyridin-3-yl)phenyl]ethyl]amino]carbonyl]-4-methyl-, monosodium salt (9CI) (CA INDEX NAME)

Na

```
415902-96-4P 415902-97-5P 415902-98-6P
IT
    415902-99-7P 415903-00-3P 415903-01-4P
    415903-02-5P 415903-05-8P 415903-07-0P
    415903-09-2P 415903-11-6P 415903-12-7P
    415903-13-8P 415903-14-9P 415903-15-0P
    415903-16-1P 415903-17-2P 415903-18-3P
    415903-19-4P 415903-20-7P 415903-22-9P
    415903-24-1P 415903-26-3P 415903-28-5P
    415903-30-9P 415903-31-0P 415903-32-1P
    415903-33-2P 415903-34-3P 415903-35-4P
    415903-36-5P 415904-25-5P 415904-26-6P
    415904-27-7P 415904-28-8P 415904-29-9P
    415904-30-2P 415904-31-3P 415904-32-4P
    415904-33-5P 415904-34-6P 415904-35-7P
    415904-36-8P 415904-37-9P 415904-39-1P
    415904-40-4P 415904-41-5P 415904-42-6P
    415904-43-7P 415904-44-8P 415904-45-9P
    415904-46-0P 415904-47-1P 415904-48-2P
    415904-49-3P 415904-50-6P 415904-51-7P
    415904-52-8P 415904-53-9P 415904-54-0P
    415904-55-1P 415904-56-2P 415904-57-3P
    415904-58-4P 415904-59-5P 415904-60-8P
    415904-61-9P 415904-62-0P 415904-63-1P
    415904-64-2P 415904-65-3P 415904-66-4P
    415904-67-5P 415904-68-6P 415904-69-7P
    415904-72-2P 415904-76-6P 415904-77-7P
    415904-78-8P 415904-79-9P 415904-80-2P
    415904-86-8P 415904-88-0P 415904-90-4P
     415904-94-8P 415905-00-9P 415905-04-3P
     415905-08-7P 415905-11-2P 415905-13-4P
     415905-17-8P 415905-19-0P 415905-23-6P
     415905-25-8P 415905-27-0P 415905-33-8P
     415905-35-0P 415905-37-2P 415905-40-7P
     415905-42-9P 415905-49-6P 415905-51-0P
     415905-53-2P 415905-55-4P 415905-57-6P
     415905-59-8P 415905-63-4P 415905-69-0P
     415905-71-4P 415905-73-6P 415905-75-8P
     415905-77-0P 415905-80-5P 415906-11-5P
```

```
415906-28-4P 415906-29-5P 415906-30-8P
    415906-31-9P 415906-38-6P 415906-39-7P
    415906-40-0P 415906-41-1P 415906-46-6P
    415906-47-7P 415906-48-8P 415906-50-2P
        (prepn. of benzimidazole derivs. as prostaglandin ep receptor
        inhibitors to treat rheumatoid arthritis)
IT
    415902-95-3P 415903-03-6P 415903-06-9P
    415903-08-1P 415903-10-5P 415903-21-8P
    415903-23-0P 415903-25-2P 415903-27-4P
    415903-29-6P 415906-27-3P 415907-59-4P
    415907-60-7P 415907-61-8P 415907-62-9P
     415907-63-0P 415907-64-1P 415907-67-4P
    415907-68-5P 415907-69-6P 415907-70-9P
    415907-72-1P 415907-74-3P 415907-75-4P
    415907-76-5P 415907-77-6P 415907-78-7P
    415907-82-3P 415907-83-4P 415907-84-5P
    415907-85-6P 415907-86-7P 415907-87-8P
    415907-88-9P 415907-89-0P 415907-90-3P
    415907-91-4P 415907-92-5P 415907-93-6P
    415907-94-7P 415907-95-8P 415907-96-9P
    415907-97-0P 415907-98-1P 415907-99-2P
    415908-00-8P 415908-01-9P 415908-04-2P
    415908-05-3P 415908-06-4P 415908-07-5P
    415908-10-0P 415908-11-1P 415908-12-2P
    415908-13-3P 415908-16-6P 415908-17-7P
    415908-18-8P 415908-19-9P 415908-22-4P
    415908-23-5P 415908-24-6P 415908-25-7P
    415908-28-0P 415908-29-1P 415908-30-4P
    415908-31-5P 415908-35-9P 415908-36-0P
    415908-38-2P 415908-39-3P 415908-41-7P
    415908-47-3P 415908-49-5P 415908-51-9P
    415908-53-1P 415908-55-3P 415908-59-7P
    415908-60-0P 415908-62-2P 415908-64-4P
    415908-65-5P 415908-68-8P 415908-69-9P
    415908-70-2P 415908-71-3P 415908-72-4P
    415908-75-7P 415908-76-8P 415908-77-9P
    415908-78-0P 415908-79-1P 415908-80-4P
    415908-81-5P 415908-86-0P 415908-87-1P
    415908-88-2P 415908-89-3P 415912-18-4P
    415912-19-5P 415912-22-0P 415912-23-1P
    415912-26-4P 415912-27-5P 415912-39-9P
    415912-40-2P 415912-41-3P 415912-42-4P
    415912-43-5P 415912-46-8P 415912-47-9P
    415912-48-0P 415912-49-1P 415912-50-4P
     415912-57-1P 415912-58-2P 415912-59-3P
     415912-60-6P 415912-61-7P 415912-65-1P
    415912-66-2P 415912-67-3P 415912-68-4P
     415912-69-5P 415912-84-4P 415914-74-8P
        (prepn. of benzimidazole derivs. as prostaglandin ep receptor
```

inhibitors to treat rheumatoid arthritis)

=> d l13 1-5 cbib abs hitstr hitrn

- L13 ANSWER 1 OF 5 HCA COPYRIGHT 2003 ACS
- 137:185916 Synthesis and properties of new electroluminescent polymers possessing both hole and electron-transporting units in the main chain. Kim, Sang Woo; Shim, Sang Chul; Jung, Byung-Jun; Shim, Hong-Ku (Center for Molecular Design and Synthesis, School of Molecular Science-BK21, Department of Chemistry, Korea Advanced Institute of Science and Technology, Yusung-Gu, Taejeon, 305-701, S. Korea). Polymer, 43(15), 4297-4305 (English) 2002. CODEN: POLMAG. ISSN: 0032-3861. Publisher: Elsevier Science Ltd..
- New EL polymers possessing both hole and electron-transporting units in the main chain are synthesized. The polymer prepd. by palladium catalyzed Heck reaction of 10 and 15 show a large wt. av. mol. wt. (Mw) (25,000) and small polydispersity index (PDI) (1.2). The oligomers synthesized by Wittig condensation have Mw of 4000 and PDI of 1.8. All the polymer and oligomers synthesized exhibit remarkable thermal stability with high decompn. temp. and high Tg as detd. by thermal gravimetric anal. (TGA) and differential scanning calorimetry (DSC) under nitrogen atm. The EL emission max. peaks of the materials prepd. are in the range of 535-560 nm corresponding to green-yellowish-green. Among the three electron-transporting moieties, the 1,3,4-oxadiazole unit shows the best electron injection and transporting property.
- IT 450944-98-6P

(electroluminescent polymers possessing both hole and electron-transporting units in the main chain)

RN 450944-98-6 HCA

CN Poly[(6-phenyl-1,3,5-triazine-2,4-diyl)-1,4-phenylene-1,2-ethenediyl-1,4-phenylene[[4-[(2-ethylhexyl)oxy]phenyl]imino]-1,4-phenylene-1,2-ethenediyl-1,4-phenylene] (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

IT 450944-98-6P

(electroluminescent polymers possessing both hole and

electron-transporting units in the main chain)

Applicants

L13 ANSWER 2 OF 5 HCA COPYRIGHT 2003 ACS

136:377202 Light-emitting device and material therefor. Okada, Hisashi; Ise, Toshihiro; Mishima, Masayuki; Taguchi, Toshiki (Fuji Photo Film Co., Ltd., Japan). U.S. Pat. Appl. Publ. US 20020055014 A1 20020509, 91 pp. (English). CODEN: USXXCO. APPLICATION: US 2001-935711 20010824. PRIORITY: JP 2000-254171 20000824; JP 2001-38718 20010215; JP 2001-236419 20010803.

GI

$$\begin{array}{c|c} - CH - CH_2 \\ \hline Ar \\ \hline N \\ \hline N \\ \hline N \\ \hline \end{array} \qquad \begin{array}{c} (R^2) m \\ \end{array} \qquad \begin{array}{c} (R^2)$$

AB Light-emitting devices comprising a pair of electrodes formed on a substrate and org. compd. layers comprising a light-emitting layer provided in between the electrodes are described in which .gtoreq.1 of the org. compd. layers comprises a heterocyclic compd. having .gtoreq.2 atoms and a phosphorescent compd.; polymers with repeating units described by the general formulas I and II (Ar = arylene or divalent heterocyclic group; R1 and R2 = independently selected H or substituent; n = 0-3; q = 0-5; and m = 0-5), which may be employed as the heterocyclic compds. in the devices, are also described. The devices may also employ polymers of heterocyclic compds. from which AR is absent. The phosphorescent compd. may be an org. metal complex.

IT 422574-76-3 422574-77-4 422574-78-5

(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle deriv. polymers for them)

RN 422574-76-3 HCA

CN Benzenamine, 4-[4-(4-ethenylphenyl)-6-phenyl-1,3,5-triazin-2-yl]-N,N-diphenyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 422574-75-2 CMF C35 H26 N4

RN 422574-77-4 HCA

CN Benzenamine, 4-[4-(4-ethenylphenyl)-6-phenyl-1,3,5-triazin-2-yl]-N,N-diphenyl-, polymer with 9-ethenyl-9H-carbazole (9CI) (CA INDEX NAME)

CM 1

CRN 422574-75-2 CMF C35 H26 N4

CM 2

CRN 1484-13-5 CMF C14 H11 N

RN 422574-78-5 HCA

CN Benzenamine, 4-[4-(4-ethenylphenyl)-6-phenyl-1,3,5-triazin-2-yl]-N,N-diphenyl-, polymer with 2-(4-ethenylphenyl)-3-phenyl-3H-imidazo[4,5-b]pyridine (9CI) (CA INDEX NAME)

CM 1

CRN 422574-75-2 CMF C35 H26 N4

CM 2

CRN 422574-61-6 CMF C20 H15 N3

IT 422574-64-9P

(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle deriv. polymers for them)

RN 422574-64-9 HCA

CN 1,3,5-Triazine, 2-(4-ethenylphenyl)-4,6-diphenyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 422574-63-8 CMF C23 H17 N3

IT 422574-76-3 422574-77-4 422574-78-5

(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle

deriv. polymers for them)

IT 422574-64-9P

(light-emitting devices with emitting layers including heterocyclic compds. and phosphorescent materials and heterocycle deriv. polymers for them)

L13 ANSWER 3 OF 5 HCA COPYRIGHT 2003 ACS

125:181108 Photographic material with polymeric UV absorber. Hagemann, Joerg; Helling, Guenter; Renner, Guenter (Agfa-Gevaert Ag, Germany). Ger. Offen. DE 19500441 Al 19960711, 23 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1995-19500441 19950110.

GI

$$(R^3)_n$$
 R^2
 $(R^1)_m$
 R^4
 R^2
 $(R^3)_p$ II

The title material comprises a support coated with multiple color photog. emulsion layers where .gtoreq.1 layers contains a polymeric UV absorber obtained by polymn. of the monomer I [R1, R3 = halogen, OH, mercapto, alkyl, aryl, alkoxy, aryloxy, acyloxy, alkylthio, arylthio, NR5R6, alkoxycarbonyl, carbamoyl, sulfamoyl; R2 = H, OH, halogen, alkyl; R4 = alkyl, alkoxy, alkylthio, aryloxy, II; R5 = H, alkyl, acyl; R6 = H, alkyl, acyl, aryl, alkoxycarbonyl, carbamoyl, sulfamoyl; m, n, p = 1-4; Z = bond] where >1 of R1, R2 and R3 and .gtoreq.1 of R1 and R4 contains ethylenically unsatd. polymerizable group. The material shows less oil building, high extinction coeff. and sweating resistance.

IT 178868-83-2P 180681-66-7P

(photog. material with polymeric UV absorber for improved sweating resistance)

RN 178868-83-2 HCA

CN 2-Propenoic acid, 2-methyl-, 2-[4-[4,6-bis[4-(1-methylpropyl)phenyl]-1,3,5-triazin-2-yl]-3-hydroxyphenoxy]ethyl ester, polymer with butyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 178868-79-6 CMF C35 H39 N3 O4

CM 2

CRN 141-32-2 CMF C7 H12 O2

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{n-BuO-C-CH----} \text{CH----} \end{array}$$

RN 180681-66-7 HCA

CN 2-Propenoic acid, 2-methyl-, 2-[4-[4,6-bis[4-(1-methylpropyl)phenyl]-1,3,5-triazin-2-yl]-3-hydroxyphenoxy]ethyl ester, polymer with ethyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 178868-79-6 CMF C35 H39 N3 O4

$$\begin{array}{c} \text{Me} \\ \text{CH-Et} \\ \\ \text{Et-CH} \\ \\ \text{N} \\ \text{N} \\ \\ \text{OH} \\ \end{array} \begin{array}{c} \text{O } \text{CH}_2 \\ \\ \text{CH}_2 - \text{CH}_2 - \text{O-C-C-Me} \\ \\ \text{OH} \\ \end{array}$$

CM 2

CRN 140-88-5 CMF C5 H8 O2

IT 178868-83-2P 180681-66-7P

(photog. material with polymeric UV absorber for improved sweating resistance)

L13 ANSWER 4 OF 5 HCA COPYRIGHT 2003 ACS

125:99940 Photographic material with improved UV-resistance. Hagemann, Joerg; Helling, Guenter; Weber, Beate (Agfa-Gevaert Ag, Germany). Ger. Offen. DE 19536376 Al 19960515, 21 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1995-19536376 19950929.

GI

$$(R^3)_n$$
 R^2
 $(R^1)_m$
 R^4
 R^4
 $R^3)_p$ II

AB In the title material contg. at least a light-sensitive Ag halide emulsion layer and at least a light-insensitive layer on a support, at least one of the layers contains an UV-absorber polymer latex obtained from homo- or copolymg. a monomer I (R1, R3 = halo, H, mercapto, alkyl, aryl, alkoxy, aryloxy, acyloxy, alkylthio, acyloxy, alkylthio, arylthio, NR5R6, alkoxycarbonyl, carbamoyl, sulfamoyl; R2 = H, OH, halo, alkyl; R4 = alkyl, alkoxy, alkylthio, aryloxy, arylthio, residue of II; R5 = H, alkyl, aryl; R6 = H, alkyl, aryl, acyl, alkoxycarbonyl, carbamoyl, sulfamoyl, sulfonyl; Z = connection site; m, n, p = 1, 2, 3, 4) and a non-polymer UV-absorber. The non-polymer UV-absorber is also claimed.

IT 178868-80-9 178868-83-2

(UV-absorber polymer of photog. material with improved UV-resistance)

RN 178868-80-9 HCA

CN 2-Propenoic acid, 2-methyl-, 2-[4-[4,6-bis[4-(1-methylpropyl)phenyl]-1,3,5-triazin-2-yl]-3-hydroxyphenoxy]ethyl ester, polymer with ethyl 2-propenoate and 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-propanesulfonic acid (9CI) (CA INDEX NAME)

CM 1

CRN 178868-79-6 CMF C35 H39 N3 O4

CM 2

CRN 15214-89-8 CMF C7 H13 N O4 S

$$\begin{array}{c} \text{O} \\ || \\ \text{NH-C-CH-CH-CH}_2 \\ || \\ \text{Me-C-CH}_2 - \text{SO}_3 \text{H} \\ || \\ \text{Me} \end{array}$$

CM 3

CRN 140-88-5 CMF C5 H8 O2

RN 178868-83-2 HCA

CN 2-Propenoic acid, 2-methyl-, 2-[4-[4,6-bis[4-(1-methylpropyl)phenyl]-1,3,5-triazin-2-yl]-3-hydroxyphenoxy]ethyl ester, polymer with butyl 2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 178868-79-6

CMF C35 H39 N3 O4

Me CH-Et

$$Me$$
 $CH-Et$
 $O-CH_2-CH_2-O-C-C-Me$
 $O-CH_2-CH_2-O-C-C-Me$

CM 2

CRN 141-32-2 CMF C7 H12 O2

IT 178868-80-9 178868-83-2

(UV-absorber polymer of photog. material with improved UV-resistance)

ANSWER 5 OF 5 HCA COPYRIGHT 2003 ACS 96:200244 Synthesis and polymerization of p-(substituted phenyl)-1,3,5-triazine monomers using imidates. Seo, Toshihiro; Hoga, Takuya; Kakurai, Toshio (Dep. High Polym. Technol., Tokyo Inst. Technol., Ookayama, 152, Japan). Nippon Kagaku Kaishi (3), 485-96 (Japanese) 1982. CODEN: NKAKB8. ISSN: 0369-4577. 2-Amino-4-(p-substituted phenyl)- and 2,4-diphenyl-6-alkenyl-1,3,5-AΒ triazines were prepd. in high yields from benzimidoylguanidines or N-benzimidoylbenzamidine with unsatd. acid chlorides. homopolymn. of these triazines and their copolymn. with Me methacrylate were studied in dioxane at 60.degree. with AIBN or at 30.degree. with PhNMe2-Bz2O2. Q Values were very large, and neg. e values decreased with increasing electron release by substituents on the Ph ring. This may be related to a neg. inductive effect and conjugation of the Ph group with a double bond through the triazine ring. Pendant 2-amino-4-phenyl- and 2,4-diphenyl-1,3,5-triazines decreased the flexibility of the polymer chain, and the softening point rose considerably with increasing triazine ring content.

Polymers contg. 2,4-diphenyltriazine rings were readily sol. in nonpolar solvents, while polymers contg. 2-amino-4-phenyltriazine rings were sol. in polar solvents. The interaction between aminotriazines of these polymers was less than that in polymers contg. guanamine rings, and the rigidity and hydrophobicity of arom. rings attached to triazine rings affected the phys. and thermal properties of the polymers.

IT 81843-46-1P 81855-82-5P 81855-83-6P

(prepn. of)

RN 81843-46-1 HCA

CN 2-Propenoic acid, 2-methyl-, methyl ester, polymer with 2-(1-methylethenyl)-4,6-diphenyl-1,3,5-triazine (9CI) (CA INDEX NAME)

CM 1

CRN 81843-45-0 CMF C18 H15 N3

$$\begin{array}{c|c} \text{Ph} & \text{CH}_2 \\ \parallel & \\ \text{C-Me} \\ \hline N & N \\ \hline \text{Ph} \end{array}$$

CM 2

CRN 80-62-6 CMF C5 H8 O2

$$^{\mathrm{H_2C}}$$
 O $^{\mathrm{H_2C}}$ $^{\mathrm{H_2C}}$ $^{\mathrm{Me}}$

RN 81855-82-5 HCA

CN 1,3,5-Triazine, 2-(1-methylethenyl)-4,6-diphenyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 81843-45-0 CMF C18 H15 N3

$$\begin{array}{c|c} \text{CH}_2 \\ \parallel \\ \text{C-Me} \\ \\ N & N \\ \\ \text{Ph} \end{array}$$

RN 81855-83-6 HCA

CN 1,3,5-Triazine, 2-ethenyl-4,6-diphenyl-, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 81854-87-7 CMF C17 H13 N3

IT 81843-46-1P 81855-82-5P 81855-83-6P (prepn. of)

=> d l18 1-27 cbib abs hitstr hitind

L18 ANSWER 1 OF 27 HCA COPYRIGHT 2003 ACS

138:18269 Synthesis of liquid-crystalline, highly luminescent .pi.-conjugated 1,3,5-triazine derivatives by palladium-catalyzed cross-coupling reaction. Lee, Chi-Han; Yamamoto, Takakazu (Chemical Resources Laboratory, Tokyo Institute of Technology, Yokohama, 226-8503, Japan). Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals, 378, 13-21 (English) 2002. CODEN: MCLCE9. ISSN: 1058-725X. Publisher: Taylor & Francis Ltd..

AB A new class of 2,4,6-triphenyl-1,3,5-triazine derivs. having long alkoxyl side chains were synthesized by a Pd(0)/Cu(I)-catalyzed C-C coupling reaction. These compds. behave as liq.-cryst. materials and show quantum yields >70% in photoluminescence.

IT 406697-93-6P 406697-94-7P 406697-95-8P 406697-96-9P

(prepn., UV-visible spectra, photoluminescence and liq. crystal

properties of)

RN406697-93-6 HCA CN

1,3,5-Triazine, 2,4,6-tris[4-[[4-(decyloxy)phenyl]ethynyl]phenyl]-(CA INDEX NAME)

PAGE 1-A

Me-
$$(CH_2)$$
 9-0

PAGE 1-B

- (CH₂)₉-Me

406697-94-7 HCA RN

1,3,5-Triazine, 2,4,6-tris[4-[[4-(dodecyloxy)phenyl]ethynyl]phenyl]-CN(9CI) (CA INDEX NAME)

PAGE 1-A $Me-(CH_2)_{11}-O$

PAGE 1-B

-- (CH₂)₁₁-Me

RN 406697-95-8 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[4-(tetradecyloxy)phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

-- (CH₂)₁₃-Me

RN 406697-96-9 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[4-(hexadecyloxy)phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-B

-- (CH₂)₁₅ - Me

IT 406697-92-5P 477705-82-1P

(prepn., UV-visible spectra, photoluminescence and transition temps. of)

RN 406697-92-5 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[4-(hexyloxy)phenyl]ethynyl]phenyl]-(9CI) (CA INDEX NAME)

PAGE 1-A

Me-
$$(CH_2)_5$$
-0

 $C = C$
 N
 N
 $C = C$

PAGE 1-B

- (CH₂)₅-Me

____O─ (CH₂)₅− Me

RN 477705-82-1 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[(4-[(2S)-2-methylbutoxy]phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-B

CC 75-11 (Crystallography and Liquid Crystals) Section cross-reference(s): 28, 73

ST synthesis liq crystal behavior **luminescent** triazine deriv; palladium catalyzed cross coupling reaction triazine deriv mesophase

IT Luminescence

(of .pi.-conjugated triazine deriv. liq. crystals)

IT Cross-coupling reaction

Liquid crystals

(synthesis and thermal behavior of highly luminescent

.pi.-conjugated triazine derivs. formed by palladium-catalyzed cross-coupling reaction)

IT 406697-93-6P 406697-94-7P 406697-95-8P 406697-96-9P

(prepn., UV-visible spectra, photoluminescence and liq. crystal properties of)

IT 406697-92-5P 477705-82-1P

(prepn., UV-visible spectra, photoluminescence and transition temps. of)

IT 7440-05-3, Palladium, uses

(synthesis and thermal behavior of highly **luminescent** .pi.-conjugated triazine derivs. formed by palladium-catalyzed cross-coupling reaction)

L18 ANSWER 2 OF 27 HCA COPYRIGHT 2003 ACS

137:331166 Conjugated polymers, their preparation and uses. O'Dell, Richard; Towns, Carl; McKiernan, Mary (Cambridge Display Technology Limited, UK). PCT Int. Appl. WO 2002083760 A2 20021024, 26 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG,

TR. (English). CODEN: PIXXD2. APPLICATION: WO 2002-GB1585 20020410. PRIORITY: GB 2001-9108 20010411.

The polymers comprise a first repeating unit of ArX2 (where Ar comprises a substituted or unsubstituted heteroaryl group, and each X comprises a substituted or unsubstituted aryl or heteroaryl group) and a second repeating unit that is adjacent to the first repeating unit, wherein each X that is part of a main body of the polymer backbone is directly conjugated to the second repeating unit. The polymers are useful for optical devices (e.g., electroluminescent devices), emissive materials, electron-transporting materials, and hole-transporting materials. Thus, a polymer was prepd. by polymn. of a bis(4-bromophenyl)triazine deriv. with 9,9-dioctylfluorene diester.

IT 473442-05-6D, polymers with 9,9-dioctylfluorene diester (conjugated polymers for optical devices)

RN 473442-05-6 HCA

CN 1,3,5-Triazine, 2,4-bis(4-bromophenyl)-6-[4-(1-methylpropyl)phenyl]-(9CI) (CA INDEX NAME)

IC ICM C08G061-00

CC 74-13 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
Section cross-reference(s): 73

ST conjugated polymer **electroluminescent** device; hole transporting material conjugated polymer

IT Electroluminescent devices

(conjugated polymers for electroluminescent devices)

IT 123863-99-0D, 9,9-Dioctylfluorene, diesters, polymers with bis(bromophenyl)triazine 473442-05-6D, polymers with 9,9-dioctylfluorene diester

(conjugated polymers for optical devices)

L18 ANSWER 3 OF 27 HCA COPYRIGHT 2003 ACS

137:125184 Preparation of **fluorescent** triazine-containing tristyryl compounds and their intermediate trialdehyde. Murata, Yukichi (Mitsubishi Chemical Corp., Japan). Jpn. Kokai Tokkyo Koho JP 2002212170 A2 20020731, 6 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2001-8657 20010117.

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Triazine-contg. tristyryl compds. I (Ar1, Ar2 = arom. group), useful as fluorescent brighteners, blue electroluminescent materials, etc. (no data), are prepd. by condensation of 2,4,6-tris(p-formylphenyl)triazine (II) with CH2Ar1Ar2 (Ar1, Ar2 = same as I) or their derivs. 2,4,6-Tris(p-methylphenyl)triazine was oxidized by CrO3 to give II, which (2 g) was treated with Ph2CHP(O)(OEt)2 in DMSO in the presence of tert-BuOK at room temp. for 2 h to give 0.9 g I (Ar1 = Ar2 = Ph) showing .lambda.max 360 nm in absorption spectrum and 454 nm in fluorescence spectrum.
- IT 443922-07-4P 443922-08-5P 443922-09-6P 443922-10-9P 443922-11-0P 443922-12-1P
 - 443922-13-2P 443922-14-3P

(prepn. of **fluorescent** triazine-contg. tristyryl compds. and their intermediate trialdehyde)

- RN 443922-07-4 HCA
- CN 1,3,5-Triazine, 2,4,6-tris[4-(2,2-diphenylethenyl)phenyl] (9CI) (CA INDEX NAME)

- RN 443922-08-5 HCA
- CN 1,3,5-Triazine, 2,4,6-tris[4-[2,2-bis(4-methylphenyl)ethenyl]-(9CI) (CA INDEX NAME)

RN 443922-09-6 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-[2,2-bis(4-methoxyphenyl)ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 443922-10-9 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(2-naphthalenyl)-2-phenylethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 443922-11-0 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(9-anthracenyl)-2-phenylethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 443922-12-1 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[2-phenyl-2-(2-thienyl)ethenyl]phenyl]-(9CI) (CA INDEX NAME)

RN 443922-13-2 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-(2,2-di-2-thienylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 443922-14-3 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(2-furanyl)-2-phenylethenyl]phenyl]- (9CI) (CA INDEX NAME)

IC ICM C07D251-24

ICS C09B057-00; C09K011-06

CC 28-19 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 73

ST triazine tristyryl prepn fluorescent brightener electroluminescence; blue electroluminescence tristyryl triazine prepn; formylphenyltriazine prepn condensation methylene diaryl

IT Electroluminescent devices

(blue-emitting; prepn. of **fluorescent** triazine-contg. tristyryl compds. and their intermediate trialdehyde)

IT Fluorescent brighteners

(prepn. of **fluorescent** triazine-contg. tristyryl compds. and their intermediate trialdehyde)

6726-45-0 27329-60-8

(prepn. of **fluorescent** triazine-contg. tristyryl compds. and their intermediate trialdehyde)

IT 443922-06-3P

IT

(prepn. of **fluorescent** triazine-contg. tristyryl compds. and their intermediate trialdehyde)

IT 443922-07-4P 443922-08-5P 443922-09-6P

443922-10-9P 443922-11-0P 443922-12-1P

443922-13-2P 443922-14-3P

(prepn. of **fluorescent** triazine-contg. tristyryl compds. and their intermediate trialdehyde)

L18 ANSWER 4 OF 27 HCA COPYRIGHT 2003 ACS

136:301731 Dye fixing element for diffusion-transfer photography.
Irita, Kiyoshi (Fuji Photo Film Co., Ltd., Japan). Jpn. Kokai
Tokkyo Koho JP 2002107891 A2 20020410, 38 pp. (Japanese). CODEN:

JKXXAF. APPLICATION: JP 2000-300636 20000929.

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- The invention relates to a dye fixing element for diffusion-transfer photog. with excellent light fastness without deteriorating its whiteness. The dye fixing element is made up of a mordant represented by I and/or II (R12,22 = H, alkyl; Y1,2 = substituent; X = Cl, Br, I, OH; Z = 5-7-membered heterocyclyl; R13,23 = H, Me, Et, halo), a fluorescent bleaching agent, a UV-blocking agent. A UV-blocking layer contg. the UV-blocking agent has a UV transmittance .ltoreq.30% at 320-350 nm and .gtoreq.70% at .gtoreq.370 nm.
- IT 409065-06-1

(UV absorber; Dye fixing element for diffusion-transfer photog.)

RN 409065-06-1 HCA

CN Benzeneethanol, 4-[4,6-bis(2,4-dimethylphenyl)-1,3,5-triazin-2-yl]-.alpha.-(2-ethylbutoxy)-3-hydroxy- (9CI) (CA INDEX NAME)

- IC ICM G03C008-40
 - ICS G03C008-56
- CC 74-2 (Radiation Chemistry, Photochemistry, and Photographic and Other Reprographic Processes)
- IT 3864-99-1 **409065-06-1**

(UV absorber; Dye fixing element for diffusion-transfer photog.)

L18 ANSWER 5 OF 27 HCA COPYRIGHT 2003 ACS

135:160421 Synthesis and characterization of a new class of liquid-crystalline, highly luminescent molecules containing a 2,4,6-triphenyl-1,3,5-triazine unit. Lee, C.-H.; Yamamoto, T. (Chemical Resources Laboratory, Tokyo Institute of Technology, Midori-ku, Yokohama, 226-8503, Japan). Tetrahedron Letters, 42(24), 3993-3996 (English) 2001. CODEN: TELEAY. ISSN:

0040-4039. Publisher: Elsevier Science Ltd..

- AB A new class of 2,4,6-triphenyl-1,3,5-triazine derivs. having long alkoxyl side chains were synthesized by a Pd(0)/Cu(I)-catalyzed C-C coupling reaction. These compds. behave as liq.-cryst. materials and show quantum yields >50% in photoluminescence.
- IT 352432-28-1P 352432-29-2P

(prepn. and liq. crystal properties and luminescence of)

- RN 352432-28-1 HCA
- CN 1,3,5-Triazine, 2,4,6-tris[4-[[3,4-bis(decyloxy)phenyl]ethynyl]pheny 1]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$Me^{-(CH_2)} = 0$$
 $O^{-(CH_2)} = Me$
 $O^{-(CH_2)} = 0$
 $O^{-(CH_$

$$\sim$$
 0- (CH₂)₉-Me

RN 352432-29-2 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[3,4-bis(undecyloxy)phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)

 ${\tt Me}$

$$-$$
 0- (CH₂)₁₀-Me

IT 352432-27-0P 352432-32-7P

(prepn. and solid-state polymorphism and **luminescence** of)

RN 352432-27-0 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[3,4-bis(nonyloxy)phenyl]ethynyl]pheny l]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$\begin{array}{c} \text{Me}-\text{(CH}_2)_8-\text{O} \\ \text{C} \\ \text{C}$$

$$\sim$$
 O- (CH₂)₈-Me

RN 352432-32-7 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[3,4-bis(tetradecyloxy)phenyl]ethynyl] phenyl]- (9CI) (CA INDEX NAME)

$$Me-(CH_2)_{13}-O$$
 $C=C$
 N
 N
 N
 $C=C$
 N
 N
 N

Me-

$$--$$
 0- (CH₂)₁₃-Me

IT 352432-30-5P 352432-31-6P

(prepn. and thermal behavior and luminescence of)

RN 352432-30-5 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[3,4-bis(dodecyloxy)phenyl]ethynyl]phe nyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

$$-$$
 O- (CH₂)₁₁-Me

RN 352432-31-6 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[[3,4-bis(tridecyloxy)phenyl]ethynyl]phenyl]- (9CI) (CA INDEX NAME)

PAGE 1-A C≡ C

$$Me-(CH_2)_{12}-O$$
 $C=C$
 $O-(CH_2)_{12}-Me$
 $O-(CH_2)_{12}-Me$
 $O-(CH_2)_{12}-Me$

Me-

$$-$$
 O- (CH₂)₁₂-Me

CC 75-11 (Crystallography and Liquid Crystals) Section cross-reference(s): 28, 73

ST phenyltriazine alkoxy deriv prepn liq crystal luminescence

IT Luminescence

(of triphenyltriazine derivs. having long alkoxyl side chains)

IT 352432-28-1P 352432-29-2P

(prepn. and lig. crystal properties and luminescence
of)

IT 352432-27-0P 352432-32-7P

(prepn. and solid-state polymorphism and luminescence of)

IT 352432-30-5P 352432-31-6P

(prepn. and thermal behavior and luminescence of)

L18 ANSWER 6 OF 27 HCA COPYRIGHT 2003 ACS

134:340526 Triazine compositions. Hu, Nan-Xing; Popovic, Zoran D.; Ong, Beng S.; Aziz, Hany (Xerox Corporation, USA). U.S. US 6229012 Bl 20010508, 19 pp., Cont.-in-part of U.S. 6,057,048. (English). CODEN: USXXAM. APPLICATION: US 2000-489527 20000121. PRIORITY: US 1998-164753 19981001.

AΒ Triazine compds. are described by the general formula I (Ar1, Ar2, Ar3, and Ar4 = independently selected aryl and/or aliph. groups; R1 and R2 independently selected H, alkyl, aryl, alkoxy, halo, and cyano; and L is a divalent group which may be absent). Use of the compds. in **electroluminescent** devices is indicated.

IT 337953-32-9P

(triazine derivs.)

337953-32-9 HCA RN

1,3,5-Triazine, 2,2'-[1,1'-biphenyl]-4,4'-diylbis[4,6-bis[4-(1,1-CN dimethylethyl)phenyl] - (9CI) (CA INDEX NAME)

IT 337953-26-1

(triazine derivs.)

RN 337953-26-1 HCA

1,3,5-Triazine, 2,2'-(9,9-diethyl-9H-fluorene-2,7-diyl)bis[4,6-CN diphenyl- (9CI) (CA INDEX NAME)

IC ICM C07D251-24

544180000 NCL

28-19 (Heterocyclic Compounds (More Than One Hetero Atom)) CC Section cross-reference(s): 73

electroluminescent triazine deriv ST

IT Phosphors

(electroluminescent; triazine derivs.)

Electroluminescent devices IT

(triazine compns. for)

2085-33-8, Tris(8-hydroxyquinolinato)aluminum 50926-11-9, Indium IT

tin oxide 58328-31-7 123847-85-8 182947-41-7, Magnesium 90, silver 10 (atomic)

(triazine compns. in electroluminescent devices with)

IT 266349-83-1P 266349-84-2P 266349-85-3P 266349-86-4P 337953-32-9P

(triazine derivs.)

IT 266349-88-6 336624-16-9 336624-17-0 336624-18-1 336624-19-2 337953-25-0 **337953-26-1** 337953-27-2 337953-28-3 337953-29-4 337953-30-7 337953-31-8 (triazine derivs.)

L18 ANSWER 7 OF 27 HCA COPYRIGHT 2003 ACS

134:333997 Triazine derivatives and **electroluminescent** (**EL**) devices using them. Esteghamatian, Mohammad; Hu,
Nan-xing; Popovic, Zoran D.; Hor, Ah-mee; Ong, Beng S. (Xerox
Corporation, USA). U.S. US 6225467 B1 20010501, 21 pp. (English).
CODEN: USXXAM. APPLICATION: US 2000-489754 20000121.

GI

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- The title triazine derivs. are described by the general formulas I-IV (Ar1-4 = independently selected aryl groups; R1, R2 = H, alkyl, aryl, alkoxy, halo, and cyano; R3, R4 = -C(R'R")-, alkylene, O, S, and -Si(R'R")-; and R' and R" = H, alkyl, alkoxy, and aryl).

 Electroluminescent devices employing the derivs. as electron transport layers are also described.

IT 266349-90-0

(triazine derivs. and **electroluminescent** devices using them in electron transport layers)

RN 266349-90-0 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4-(3-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)

IT 6888-33-1P

(triazine derivs. and **electroluminescent** devices using them in electron transport layers)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

IC ICM C07D251-24 ICS H05B033-14

NCL 544180000

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 29, 76

ST triazine deriv **electroluminescent** device electron transport layer

IT Phosphors

(electroluminescent; triazine derivs. and electroluminescent devices using them in electron transport layers)

IT **Electroluminescent** devices

(triazine derivs. and **electroluminescent** devices using them in electron transport layers)

IT 2085-33-8, Tris(8-hydroxyquinolinato)aluminum 12614-86-7 50926-11-9, Indium tin oxide 58328-31-7 123847-85-8 266349-86-4 **266349-90-0** 336624-13-6 336624-14-7 336624-15-8 336624-16-9 336624-17-0 336624-18-1 336624-19-2 (triazine derivs. and electroluminescent devices using them in electron transport layers)

IT **6888-33-1P** 31274-51-8P 266349-83-1P 266349-84-2P 266349-85-3P

(triazine derivs. and **electroluminescent** devices using them in electron transport layers)

IT 100-47-0, Benzonitrile, reactions 104-85-8, p-Tolunitrile 620-22-4 2351-37-3, 4,4'-Biphenyldicarbonyl chloride 2920-38-9, 4-Biphenylcarbonitrile 14002-51-8, 4-Biphenylcarbonyl chloride 16107-88-3

(triazine derivs. and **electroluminescent** devices using them in electron transport layers)

L18 ANSWER 8 OF 27 HCA COPYRIGHT 2003 ACS

132:327508 Electroluminescent (EL) devices. Hu,
Nan-xing; Esteghamatian, Mohammad; Qi, Yu; Popovic, Zoran D.; Ong,
Beng S.; Hor, Ah-mee (Xerox Corp., USA). U.S. US 6057048 A
20000502, 31 pp. (English). CODEN: USXXAM. APPLICATION: US
1998-164753 19981001.

AB Electroluminescent devices comprising an anode, a hole transporting layer, a light emitting layer, and a cathode are described in which the light emitting layer contains a component described by the general formula I (Ar1-4 = independently selected aryl or aliph. groups; R1 and R2 = independently selected from hydrogen, aliph., halogen, and cyano; L = a conjugated bivalent linking group; and n = 0-3); the compds. may serve as hosts for selected fluorescent dyes.

IT 266349-92-2 266349-93-3 266349-97-7

(electroluminescent devices using triazine derivs.)

RN 266349-92-2 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis([1,1'-biphenyl]-3-yl)- (9CI) (CA INDEX NAME)

RN 266349-93-3 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis(3-methoxyphenyl)- (9CI) (CA INDEX NAME)

RN 266349-97-7 HCA

CN 1,3,5-Triazine, 4-[4-[2-[4'-(4,6-diphenyl-1,3,5-triazin-2-yl)[1,1'-biphenyl]-4-yl]ethenyl]phenyl]-2,6-diphenyl- (9CI) (CA INDEX NAME)

IT 6888-33-1P 266349-90-0P 266349-91-1P (electroluminescent devices using triazine derivs.)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 266349-90-0 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4-(3-methylphenyl)-6-phenyl- (9CI) (CA INDEX NAME)

RN 266349-91-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis([1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)

IC ICM H05B033-14

NCL 428690000

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

Section cross-reference(s): 28, 76

ST triazine deriv electroluminescent device

IT Electroluminescent devices

Electroluminescent devices

(electroluminescent devices using triazine derivs.)

IT 91-64-5, Coumarin 12798-95-7 37271-44-6 58328-31-7

123847-85-8 266349-86-4 266349-87-5 266349-88-6 266349-89-7

266349-92-2 266349-93-3 266349-94-4

266349-95-5 266349-96-6 **266349-97-7** 266349-98-8

266349-99-9 266350-00-9 266350-01-0

(electroluminescent devices using triazine derivs.)

IT 198-55-0, Perylene 517-51-1, Rubrene 1499-10-1,

9,10-Diphenylanthracene. 2085-33-8, Tris(8-

hydroxyquinolinato)aluminum 16043-42-8 19205-19-7,

N,N'-Dimethylquinacridone 222402-84-8 266349-59-1 266349-61-5 266349-63-7

(electroluminescent devices using triazine derivs.)

IT 6888-33-1P 266349-83-1P 266349-84-2P 266349-85-3P 266349-90-0P 266349-91-1P

200349-90-02 200349-91-12

(electroluminescent devices using triazine derivs.)

IT 95-50-1, 1,2-Dichlorobenzene 100-47-0, Benzonitrile, reactions

104-85-8, p-Tolunitrile 620-22-4 2351-37-3, 4,4'-Biphenyldicarbonyl chloride 7704-34-9, Sulfur, reactions 16107-88-3

(electroluminescent devices using triazine derivs.)

L18 ANSWER 9 OF 27 HCA COPYRIGHT 2003 ACS
124:246169 Organic field-effect **electroluminescent** device.
Sato, Yoshiharu (Mitsubishi Kagaku Kk, Japan). Jpn. Kokai Tokkyo

Koho JP 08012967 A2 19960116 Heisei, 9 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1994-147730 19940629.

GI

$$Ar^{1}$$
 N
 $CH = CH$
 N
 Ar^{2}
 Ar^{4}
 I

The device has an org. light-emitting layer contg. a 4,4'-bis(triazinylstilbene) deriv. described by the general formula I (Ar1-4 = aryl, biphenyl, arom. heterocyclic group; Ar1-4 may be substituted) and a hole-transporting layer between an anode and a cathode on a substrate. The device showed high and stable luminance.

IT 6888-33-1

(field-effect electroluminescent device having bis(triazinylstilbene) deriv. light-emitting layer with high and stable luminance)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

IC ICM C09K011-06 ICS H05B033-14

CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 28

ST triazinyl stilbene electroluminescent device

IT **Electroluminescent** devices

(field-effect **electroluminescent** device having bis(triazinylstilbene) deriv. **light-emitting** layer with high and stable luminance)

IT 6888-33-1

(field-effect **electroluminescent** device having bis(triazinylstilbene) deriv. **light-emitting** layer with high and stable luminance)

- L18 ANSWER 10 OF 27 HCA COPYRIGHT 2003 ACS
- 117:214164 Vinyl chloride polymer **fluorescent** films for agricultural use. Nakai, Takemoto; Ito, Yoshiko (Mitsubishi Kasei Vinyl K. K., Japan). Jpn. Kokai Tokkyo Koho JP 04144618 A2 19920519 Heisei, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1990-267746 19901005.

GΙ

- AB Title films contain UV-excitable fluorescent substances and .gtoreq.1 amide selected from N,N'-dioleyladipamide (I) and ethylenebislaurylamide or .gtoreq.1 urea compd. selected from xylylenebisstearylurea and toluylenebisstearylurea. Thus, a film prepd. from a mixt. of PVC 100, DOP 42, Epikote 828 4, Ca-Zn stabilizers 5, sorbitan monopalmitate 1.5, fluorescent agent (II) 0.5, and I 0.4 part was exposed outdoors to show fluorescence intensity 30% initially, 19% after 1 mo, 10% after 3 mo, and 4% after 5 mo.
- IT 67014-59-9

(fluorescent substances, PVC films contg. amides and, with good weatherability, for agricultural uses)

- RN 67014-59-9 HCA
- CN Benzoxazole, 2-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]-5,6-dimethyl- (9CI) (CA INDEX NAME)

- IC ICM A01G009-14
 - ICS A01G013-02; C08K005-20; C08K005-21; C08L027-06

CC 38-3 (Plastics Fabrication and Uses)

ST fluorescent film vinyl chloride polymer;
toluylenebisstearylurea fluorescent vinyl film;
xylylenebisstearyl urea fluorescent vinyl film;
ethylenebislaurylamide fluorescent vinyl film; benzoxazole
fluorescent PVC film agriculture; oleyladipamide PVC
fluorescent film; weather resistance fluorescent
film PVC

IT Fluorescent substances

(PVC films contg. amides and, with good weatherability, for agricultural uses)

IT Greenhouses

(fluorescent films for, vinyl chloride polymers contg. urea derivs. or amides as, with good weatherability)

TT 7003-56-7, Ethylenebislaurylamide 85888-37-5, N,N'-Dioleyladipamide 91835-70-0 91835-71-1 (PVC films contg. **fluorescent** substances and, with good weatherability, for agricultural uses)

IT 9002-86-2, PVC

(films, **fluorescent**, weather-resistant, contg. amides or urea compds., for agriculture)

IT 81-83-4D, Naphthalimide, derivs. 7128-64-5 **67014-59-9**138647-80-0 138647-82-2 139106-96-0, Lumogen F Violet 570
144232-60-0 144232-61-1
(**fluorescent** substances, PVC films contg. amides and,

(**fluorescent** substances, PVC films contg. amides and with good weatherability, for agricultural uses)

L18 ANSWER 11 OF 27 HCA COPYRIGHT 2003 ACS

116:107817 Vinyl chloride polymer **fluorescent** films for agricultural uses. Nakai, Takemoto; Tanaka, Keiji (Mitsubishi Kasei Vinyl K. K., Japan). Jpn. Kokai Tokkyo Koho JP 03198721 A2 19910829 Heisei, 4 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1989-338987 19891227.

The title films, with stable **fluorescent** energy, are prepd. from the title polymers, benzooxazole derivs. as **fluorescent** agents, and Mg compd. fine particles. Thus, a PVC compn. contg. 0.5 phr I and 2 phr MgO was calendered to give a 0.1-mm film having **fluorescent** strength (increased light strength based on sun light) 30, 25, and 15%, initially, after 1 mo, and after 3 mo, resp.; vs. 30, 8, and 0, resp., for a film without MgO.

IT 67014-59-9

(fluorescent agents, PVC films contg. magnesium compds. and, for fluorescent agricultural films)

RN 67014-59-9 HCA

CN Benzoxazole, 2-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]-5,6-dimethyl- (9CI) (CA INDEX NAME)

IC ICM A01G009-14

ICS A01G013-02; C08J005-18

ICI C08L027-06

CC 38-3 (Plastics Fabrication and Uses)

Section cross-reference(s): 19

ST benzooxazole deriv **fluorescent** PVC film; magnesium oxide **fluorescent** PVC film; agriculture film **fluorescent** PVC

IT Fluorescent substances

(PVC films contg. benzooxazole deriv. and magnesium compds. as, for **fluorescent** agricultural films)

IT Agriculture and Agricultural chemistry

(films for use in, of PVC contg. benzooxazole deriv. and magnesium compds. as, with stable **fluorescent**)

IT 546-93-0, Magnesium carbonate 1309-42-8, Magnesium hydroxide 1309-48-4, Magnesium oxide (MgO), uses 69048-27-7 (PVC films contg. fluorescent agents and, for fluorescent agricultural films)

IT 9002-86-2, PVC

(films, contg. benzooxazole deriv. and magnesium compds., for fluorescent agricultural films)

IT 7128-64-5 **67014-59-9** 138647-80-0 138647-81-1

138647-82-2

(fluorescent agents, PVC films contg. magnesium compds. and, for fluorescent agricultural films)

L18 ANSWER 12 OF 27 HCA COPYRIGHT 2003 ACS

111:92325 Plastic foils with improved light transmission for agriculture. Ebner, Guido; Hefti, Heinz (Ciba-Geigy A.-G., Switz.).

Ger. Offen. DE 3818986 A1 19881222, 10 pp. (German). CODEN:
GWXXBX. APPLICATION: DE 1988-3818986 19880603. PRIORITY: CH
1987-2142 19870605.

AB Transparent foils for improvement of the rate of photosynthesis in plants contain a **fluorescent** compd. that absorbs at 300-400 nm and shows **fluorescence** at 430-470 nm.

Application of 0.1% 2,5-benzoxazol-2-ylthiophene to a polyester foil

increased light transmission at 430 and 440 nm, by 30 and 40%, resp. Potted water cress exposed in the dark to UV light showed normal development when wrapped into this foil. In the absence of the **fluorescent** compd., the foil had little effect, and growth was unsatisfactory.

IT 6568-89-4

(light transmission improvement by, in agricultural plastic foils)

RN 6568-89-4 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

IC ICM C09B023-00

ICS C09B023-14; C09B023-16; C09B023-12; C09K011-00; C09K011-02; D06L003-12; B41M005-26; A01G009-14

CC 5-3 (Agrochemical Bioregulators)

Section cross-reference(s): 11, 38

ST plastic foil fluorescent substance light agriculture

IT Acrylic polymers, biological studies

Plastics

Polyamides, biological studies

Polyesters, biological studies

(fluorescent substances-contg. foils of, with improved light transmission, for agriculture)

IT Agriculture and Agricultural chemistry

(fluorescent substances-contg. plastic sheets in, for improved light transmission)

IT Fluorescent substances

(light transmission improvement by, in agricultural plastic foils)

IT Alkenes, polymers

(polymers, fluorescent substance-contg. films of, with improved light transmission, for agriculture)

IT 9004-35-7

(fluorescent substance-contg. films of, with improved light transmission, for agriculture)

IT 9002-86-2, Poly(vinyl chloride) 9003-53-6, Polystyrene 9004-34-6, Cellulose, biological studies (fluorescent substances-contg. foils of, with improved light transmission, for agriculture)

IT 91-20-3D, Naphthalene, derivs. 91-64-5D, 2H-1-Benzopyran-2-one, 1533-45-5 2866-43-5 1041-00-5 3333-62-8 6394-12-3 6568-89-4 7128-64-5 16143-18-3 23743-30-8 40470-68-6 85130-93-4 122063-81-4 122210-86-0 (light transmission improvement by, in agricultural plastic foils)

L18 ANSWER 13 OF 27 HCA COPYRIGHT 2003 ACS
97:183951 Correction of: 96:53843 4-Heterocyclyl-4'-vinylstilbenes.
Burdeska, Kurt; Kabas, Guglielmo; Weber, Kurt (Ciba-Geigy A.-G.,
Switz.). Eur. Pat. Appl. EP 31796 A2 19810930, 94 pp. DESIGNATED
STATES: R: CH, DE, FR, GB, IT. (English). CODEN: EPXXDW.
APPLICATION: EP 1980-810393 19801215. PRIORITY: CH 1979-11402
19791221; CH 1980-7008 19800918.

GΙ

AB Compds. of general structure I are prepd., where R is a monocyclic 5- or 6-membered arom. heterocyclic group (optionally with 1 or 2 fused benzene rings), a bicyclic 9-membered arom. heterocyclic group, Ph, CN, carboxy, alkoxycarbonyl, alkylsulfonyl, or arylsulfonyl; R1 = H or alkyl; R2 = H, alkyl, alkoxycarbonyl, carbamoyl, sulfonamido, alkenyl, carboxy, alkylsulfonyl, arylsulfonyl, aralkylsulfonyl, CN, sulfo, or dialkoxyphosphinyl; R3 = H, alkyl, or alkenyl; and only one of R2 and R3 can be H. I are esp. useful as fluorescent whiteners for fibers and plastics. Over 100 addnl. I were prepd. by the same or similar methods. Thus, condensation of 2-[4-[(diethoxyphosphinyl)methyl]phe nyl-4,6-dimethoxypyrimidine [79382-97-1] with 4-HCOC6H4CH:CHCO2Me [7560-50-1] in DMF in the presence of NaOMe gave cryst. II [79381-32-1], a **fluorescent** whitener for polyester textiles.

ΙΙ

IT 79381-59-2P 79381-60-5P

(manuf. of, as **fluorescent** brightener for fibers and plastics)

RN 79381-59-2 HCA

CN 2-Propenenitrile, 3-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 79381-60-5 HCA

CN 2-Propenoic acid, 3-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

ICI C07D471-04, C07D249-00, C07D221-00; C07D498-04, C07D263-00,

CC 41-10 (Dyes, Fluorescent Brighteners, and Photographic Sensitizers)

ST heterocyclylvinylstilbene fluorescent whitener; vinylstilbene heterocyclic fluorescent whitener

IT Acetate fibers, uses and miscellaneous

Plastics

Polyamide fibers, uses and miscellaneous Polyester fibers, uses and miscellaneous

(fluorescent brighteners for,

heterocyclylvinylstilbenes as)

IT Fluorescent brighteners

(heterocyclylvinylstilbenes, for plastics and synthetic fibers)

IT 623-27-8

(condensation reactions of, in **fluorescent** brightener synthesis)

IT 9002-86-2 9003-53-6 25038-59-9, uses and miscellaneous (fluorescent brighteners for, heterocyclylvinylstilbenes as)

IT 79381-32-1P 79381-33-2P 79381-34-3P 79381-35-4P 79381-36-5P

L18 ANSWER 14 OF 27 HCA COPYRIGHT 2003 ACS
96:53843 4-Heterocyclyl-4'-vinylstilbenes. Burdeska, Kurt; Kabas,
Guglielmo; Weber, Kurt (Ciba-Geigy A.-G., Switz.). Eur. Pat. Appl.
EP 31796 A2 19810708, 94 pp. DESIGNATED STATES: R: CH, DE, FR, GB,
IT. (German). CODEN: EPXXDW. APPLICATION: EP 1980-810393
19801215. PRIORITY: CH 1979-11402 19791221; CH 1980-7008 19800918.
GI

$$R \longrightarrow CH = CH \longrightarrow CR^{1} = CR^{2}R^{3}$$

plastics)

MeO
$$\sim$$
 CH = CH \sim CH = CHCO₂Me \sim MeO \sim

AB Compds. of general structure I are prepd., where R is a monocyclic 5- or 6-membered arom. heterocyclic group (optionally with 1 or 2 fused benzene rings), a bicyclic 9-membered arom. heterocyclic group, Ph, CN, carboxy, alkoxycarbonyl, alkylsulfonyl, or

ΙI

arylsulfonyl; R1 = H or alkyl; R2 = H, alkyl, alkoxycarbonyl, carbonyl, sulfonyl, alkenyl, carboxy, alkylsulfonyl, arylsulfonyl, aralkylsulfonyl, CN, sulfo, or dialkoxyphosphinyl; R3 = H, alkyl, or alkenyl; and only one of R2 and R3 can be H. I are esp. useful as fluorescent whiteners for fibers and plastics. Thus, condensation of 2-[4-[(diethoxyphosphinyl)methyl]phenyl]-4,6-dimethoxypyrimidine [79382-97-1] with 4-HCOC6H4CH:CHCO2Me [7560-50-1] in DMF in the presence of NaOMe gave cryst. II [79381-32-1], a fluorescent whitener for polyester textiles. Over 100 addnl. I were prepd. by the same or similar methods.

IT 79381-59-2P 79381-60-5P

(manuf. of, as **fluorescent** brightener for fibers and plastics)

RN 79381-59-2 HCA

CN 2-Propenenitrile, 3-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 79381-60-5 HCA

CN 2-Propenoic acid, 3-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]-, methyl ester (9CI) (CA INDEX NAME)

- IC C07D239-26; C07D263-56; C08K005-34; C08K005-35; D06L003-12; C07C069-618; C07C121-52; C07F009-65; C07D231-12; C07D471-04; C07D498-04
- CC 41-10 (Dyes, Fluorescent Brighteners, and Photographic Sensitizers)
- ST vinylstilbene **fluorescent** whitener synthesis; stilbene **fluorescent** whitener synthesis; heterocyclylvinylstilbene **fluorescent** whitener; polyester **fluorescent** whitener
- IT 79381-32-1P 79382-27-7P (manuf. of, as a **fluorescent** brightener for fibers and

```
plastics)
IT
     79381-32-1P
                   79381-33-2P
                                  79381-34-3P
                                                 79381-35-4P
                                                                79381-36-5P
     79381-37-6P
                   79381-38-7P
                                  79381-39-8P
                                                 79381-40-1P
                                                                79381-41-2P
     79381-42-3P
                   79381-43-4P
                                  79381-44-5P
                                                 79381-45-6P
                                                                79381-46-7P
                                                 79381-50-3P
     79381-47-8P
                   79381-48-9P
                                  79381-49-0P
                                                                79381-51-4P
     79381-52-5P
                   79381-53-6P
                                  79381-54-7P
                                                 79381-55-8P
                                                                79381-56-9P
                   79381-58-1P 79381-59-2P 79381-60-5P
     79381-57-0P
     79381-61-6P
                   79381-62-7P
                                  79381-63-8P
                                                 79381-64-9P
                                                                79381-65-0P
                   79381-67-2P
                                  79381-68-3P
                                                 79381-69-4P
                                                                79381-70-7P
     79381-66-1P
                                                 79381-74-1P
                   79381-72-9P
                                  79381-73-0P
     79381-71-8P
                                                                79381-75-2P
     79381-76-3P
                   79381-77-4P
                                  79381-78-5P
                                                 79381-79-6P
                                                                79381-80-9P
     79381-81-0P
                   79381-82-1P
                                  79381-83-2P
                                                 79381-84-3P
                                                                79381-85-4P
                                  79381-88-7P
     79381-86-5P
                   79381-87-6P
                                                 79381-89-8P
                                                                79381-90-1P
     79381-91-2P
                   79381-92-3P
                                  79381-93-4P
                                                 79381-94-5P
                                                                79381-95-6P
     79381-96-7P
                   79381-97-8P
                                  79381-98-9P
                                                 79381-99-0P
                                                                79382-00-6P
                                                 79382-04-0P
                                                                79382-05-1P
     79382-01-7P
                   79382-02-8P
                                  79382-03-9P
     79382-06-2P
                   79382-07-3P
                                  79382-08-4P
                                                 79382-09-5P
                                                                79382-10-8P
                   79382-12-0P
                                  79382-13-1P
                                                 79382-14-2P
                                                                79382-15-3P
     79382-11-9P
                   79382-17-5P
                                  79382-18-6P
                                                 79382-19-7P
                                                                79382-20-0P
     79382-16-4P
                                  79382-23-3P
                                                 79382-24-4P
                                                                79382-25-5P
     79382-21-1P
                   79382-22-2P
                                  79382-29-9P
                                                 79382-30-2P
                                                                79382-31-3P
     79382-26-6P
                   79382-28-8P
     79382-32-4P
                   79382-33-5P
                                  79382-34-6P
                                                 79382-35-7P
                                                                79382-36-8P
     79382-37-9P
                   79382-38-0P
                                  79382-39-1P
                                                 79382-40-4P
                                                                79382-41-5P
     79395-99-6P
        (manuf. of, as fluorescent brightener for fibers and
```

L18 ANSWER 15 OF 27 HCA COPYRIGHT 2003 ACS
89:112426 Fluorescent dyes. Eckstein, Udo; Harnisch, Horst
(Bayer A.-G., Fed. Rep. Ger.). Ger. Offen. DE 2650456 19780511, 38
pp. (German). CODEN: GWXXBX. APPLICATION: DE 1976-2650456
19761104.

plastics)

Ι

AB Fluorescent dyes are prepd. which have general structure I, where R and R1 = halogen, OH, amino, alkoxy, aryloxy, alkyl- or arylthio, acylamino, alkyl, or aryl, X = 0, S, or NR2 (R2 = H, alkyl, aryl, acyl) rings A and B can contain nonchromophoric substituents, and ring A also can contain 1 or 2 fused carbocylic I are useful as fluorescent whiteners for synthetic fibers and plastics. Thus, reaction of 2-(chloromethyl)-5-methylbenzoxazole [41014-44-2] with (MeO)3P in DMF and treatment of the product with 4,6-dimethoxy-2-(4formylphenyl)-1,3,5-triazine [67014-40-8] in the presence of NaOMe [67014-61-3], which showed a deep blue fluorescence in DMF and a fast, strong whitening effect when incorporated in polyester. Other I were prepd. similarly or by condensing triazinylcinnamoyl chlorides with o-substituted arom. amines followed by cyclization.

IT 67014-58-8P

(prepn. and reaction with aminophenols, ring closure in)
RN 67014-58-8 HCA
CN 2-Propenoyl chloride, 3-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl](9CI) (CA INDEX NAME)

IT 67014-57-7P

(prepn. and reaction with thionyl chloride)

RN 67014-57-7 HCA

CN 2-Propenoic acid, 3-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl](9CI) (CA INDEX NAME)

$$^{\text{Ph}}$$
 $^{\text{N}}$
 $^{\text{N}}$
 $^{\text{CH}}$
 $^{\text{CH}}$
 $^{\text{CH}}$
 $^{\text{CH}}$

IT 67014-54-4P 67014-56-6P 67014-59-9P 67014-60-2P

(prepn. of)

RN 67014-54-4 HCA

CN Benzoxazole, 2-[2-[4-[4,6-bis(4-methoxyphenyl)-1,3,5-triazin-2-yl]phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 67014-56-6 HCA

CN Benzothiazole, 2-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 67014-59-9 HCA

CN Benzoxazole, 2-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-

yl)phenyl]ethenyl]-5,6-dimethyl- (9CI) (CA INDEX NAME)

RN 67014-60-2 HCA

CN Benzoxazole, 5-(1,1-dimethylethyl)-2-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

IC C07D413-10

CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

ST styryl azole fluorescent whitener; triazinylstyryl fluorescent whitener; plastic fluorescent whitener; textile fluorescent whitener

IT Fluorescent brighteners

((triazinylstyryl)benzazoles, for plastics and synthetic fibers)

IT Polyester fibers, uses and miscellaneous Polypropene fibers, uses and miscellaneous (fluorescent brighteners for,

(triazinylstyryl)benzazoles as)

IT 67014-46-4 67014-47-5 67014-48-6 67014-49-7 67014-50-0

67014-51-1 67014-52-2 67066-77-7 67066-78-8 (**fluorescent** brightener, for fibers and plastics)

IT 9003-53-6

(fluorescent brighteners for,

(triazinylstyryl)benzoxazoles as)

IT 67014-45-3P

(manuf. of, as **fluorescent** brighener for fibers and plastics)

IT 67014-44-2P

(manuf. of, as **fluorescent** brightener for fibers and plastics)

IT 67014-61-3P

(manuf. of, as **fluorescent** brightener for polyester fibers)

IT 67014-58-8P

(prepn. and reaction with aminophenols, ring closure in)

IT 67014-57-7P

(prepn. and reaction with thionyl chloride)

IT 67014-42-0P 67014-54-4P 67014-56-6P

67014-59-9P 67014-60-2P

(prepn. of)

L18 ANSWER 16 OF 27 HCA COPYRIGHT 2003 ACS

80:146981 Ethylenically unsaturated heterocyclics. Siegrist, Adolf E.; Liechti, Peter; Maeder, Erwin; Guglielmetti, Leonardo; Meyer, Hans Rudolf; Weber, Kurt (Ciba-Geigy A.-G.). Patentschrift (Switz.) CH 542212 19731115, 56 pp. (German). CODEN: SWXXAS. APPLICATION: CH 1966-13745 19660923.

Two hundred twenty-five heterocyclic compds. contg. styryl or substituted styryl groups were prepd. and were used as fluorescent whitening agents for polyester fibers and were incorporated into polyester, polyamide, and polypropylene melts which were spun into fibers having good fluorescent whitening properties. Thus, 6-phenyl-2-p-tolylbenzoxazole was treated with PhCH:NHPh in DMF in the presence of KOCMe3 at 20-31.deg. to give fluorescent whitener I [6660-87-3]. Similarly fluorescent whitener (II) [16184-00-2] was prepd. by condensation of 4-biphenylcarboxaldehyde anil with 1,4,5-triphenyl-2-p-tolylimidazole in DMF in the presence of KOH.

IT 16155-78-5P 16155-79-6P 16155-80-9P

16155-81-0P 16155-82-1P 16155-83-2P

16155-84-3P 16155-85-4P 16155-86-5P

16155-87-6P 16155-88-7P 16155-89-8P

16476-98-5P

(prepn. of)

RN 16155-78-5 HCA

CN 1,3,5-Triazine, 2-[4-[2-(4-methoxyphenyl)ethenyl]phenyl]-4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 16155-79-6 HCA

CN 1,3,5-Triazine, 2-[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 16155-81-0 HCA

CN 1,3,5-Triazine, 2-[4-(1,1-dimethylethyl)phenyl]-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-82-1 HCA

CN 1,3,5-Triazine, 2-[1,1'-biphenyl]-4-yl-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-83-2 HCA

CN 1,3,5-Triazine, 2,4-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-6-phenyl- (9CI) (CA INDEX NAME)

RN 16155-84-3 HCA

CN 1,3,5-Triazine, 2,4-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-6-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-85-4 HCA

CN 1,3,5-Triazine, 2-[1,1'-biphenyl]-4-yl-4,6-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-86-5 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-87-6 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl](9CI) (CA INDEX NAME)

RN 16155-88-7 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(4-chlorophenyl)ethenyl]phenyl]-(9CI) (CA INDEX NAME)

RN 16155-89-8 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(4-methoxyphenyl)ethenyl]phenyl]-(9CI) (CA INDEX NAME)

RN 16476-98-5 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-(2-[1,1'-biphenyl]-4-ylethenyl)-2methylphenyl]- (9CI) (CA INDEX NAME)

IT 16107-90-7

(reaction of, with benzylideneaniline derivs. in the presence of base)

RN 16107-90-7 HCA

CN 1,3,5-Triazine, 2-[4-(1,1-dimethylethyl)phenyl]-4,6-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

IC C07D

CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

ST stryryl fluorescent whitener; ethylene fluorescent
whitener; heterocyclic fluorescent whitener; polyester
fiber fluorescent whitener; polyamide fiber
fluorescent whitener; polypropene fiber fluorescent
whitener

IT Polyester fibers

(fluorescent brighteners for, stilbene derivs of heterocycles as)

IT Polyamide fibers

Polypropene fibers

(**fluorescent** brighteners for, stilbene derivs. of heterocycles as)

IT Fluorescent brighteners

(stilbene derivs. of heterocycles, for polyamide, polyester and polypropene fibers)

2718-87-8P 3962-65-0P IT 1552-56-3P 6660-87-3P 6660-89-5P 10307-62-7P 14016-18-3P 14607-84-2P 16143-02-5P 10165-24-9P 16143-08-1P 16143-03-6P 16143-04-7P 16143-05-8P 16143-07-0P 16143-12-7P 16143-14-9P 16143-09-2P 16143-10-5P 16143-11-6P 16143-16-1P 16143-17-2P 16143-18-3P 16143-19-4P 16143-15-0P 16143-23-0P 16143-24-1P 16143-20-7P 16143-22-9P 16143-21-8P 16143-25-2P 16143-26-3P 16143-27-4P 16143-28-5P 16143-29-6P 16143-35-4P 16143-33-2P 16143-34-3P 16143-32-1P 16143-31-0P 16143-40-1P 16155-61-6P 16155-62-7P 16143-36-5P .16143-37-6P 16155-67-2P 16155-64-9P 16155-65-0P 16155-66-1P 16155-63-8P 16155-71-8P 16155-72-9P 16155-73-0P 16155-68-3P 16155-69-4P 16155-77-4P 16155-76-3P 16155-74-1P 16155-75-2P

16155-78-5P 16155-79-6P 16155-80-9P

16155-81-0P 16155-82-1P 16155-83-2P

```
16155-84-3P 16155-85-4P 16155-86-5P
     16155-87-6P 16155-88-7P 16155-89-8P
     16155-90-1P
                    16155-91-2P
                                   16157-10-1P
                                                 16157-11-2P
                                                                16157-12-3P
     16157-13-4P
                    16157-14-5P
                                  16157-15-6P
                                                 16157-16-7P
                                                                16157-17-8P
                    16157-19-0P
                                  16157-20-3P
                                                 16157-21-4P
     16157-18-9P
                                                                16157-22-5P
                                  16157-25-8P
                                                 16157-26-9P
     16157-23-6P
                    16157-24-7P
                                                                16157-27-0P
     16157-28-1P
                    16157-29-2P
                                  16157-30-5P
                                                 16157-31-6P
                                                                16157-32-7P
     16157-33-8P
                    16157-34-9P
                                  16157-35-0P
                                                 16157-36-1P
                                                                16157-37-2P
                    16157-39-4P
                                  16157-40-7P
                                                 16157-41-8P
                                                                16157-42-9P
     16157-38-3P
     16157-43-0P
                    16157-44-1P
                                   16157-45-2P
                                                 16157-46-3P
                                                                16157-47-4P
                    16157-49-6P
                                  16157-50-9P
                                                 16157-52-1P
                                                                16157-53-2P
     16157-48-5P
     16157-55-4P
                    16157-56-5P
                                  16157-57-6P
                                                 16157-58-7P
                                                                16177-90-5P
     16177-91-6P
                    16177-92-7P
                                  16177-93-8P
                                                 16177-94-9P
                                                                16177-95-0P
     16177-96-1P
                    16177-97-2P
                                  16177-98-3P
                                                 16177-99-4P
                                                                16178-00-0P
                                                 16178-04-4P
                                                                16178-05-5P
     16178-01-1P
                    16178-02-2P
                                  16178-03-3P
     16178-06-6P
                    16178-07-7P
                                  16178-08-8P
                                                 16178-09-9P
                                                                16178-10-2P
     16178-11-3P
                    16178-12-4P
                                  16178-13-5P
                                                 16178-14-6P
                                                                16178-15-7P
     16178-16-8P
                    16178-17-9P
                                  16178-18-0P
                                                 16178-19-1P
                                                                16178-20-4P
                                                 16178-25-9P
                                                                16178-26-0P
     16178-22-6P
                    16178-23-7P
                                  16178-24-8P
                    16178-31-7P
                                  16178-32-8P
                                                 16178-33-9P
                                                                16178-34-0P
     16178-30-6P
     16178-35-1P
                    16178-36-2P
                                   16178-37-3P
                                                 16183-96-3P
                                                                16183-97-4P
                                  16184-01-3P
                                                 16184-02-4P
                                                                16184-03-5P
     16183-98-5P
                    16184-00-2P
     16184-07-9P
                    16184-08-0P
                                  16184-09-1P
                                                 16184-10-4P
                                                                16184-12-6P
                                  16184-17-1P
                                                 16184-18-2P
                                                                16184-19-3P
                    16184-16-0P
     16184-14-8P
                                  16184-22-8P
                                                 16184-23-9P
                                                                16184-24-0P
     16184-20-6P
                    16184-21-7P
                                                                16219-27-5P
                    16184-26-2P
                                  16184-27-3P
                                                . 16219-26-4P
     16184-25-1P
                                                                16256-12-5P
     16253-65-9P
                    16253-68-2P
                                  16256-10-3P
                                                 16256-11-4P
     16256-13-6P
                    16263-16-4P
                                  16263-17-5P
                                                 16263-18-6P
                                                                16263-19-7P
                    16263-22-2P
                                  16263-23-3P
                                                 16263-24-4P
                                                                16263-25-5P
     16263-20-0P
                                                 16263-30-2P
                                                                16325-02-3P
     16263-26-6P
                    16263-28-8P
                                  16263-29-9P
                                  16443-36-0P
                                                 16445-42-4P
                                                                16445-47-9P
                    16325-04-5P
     16325-03-4P
     16445-80-0P
                    16445-81-1P
                                  16445-95-7P 16476-98-5P
     51750-24-4P
        (prepn. of)
                                                      3682-80-2
                                                                   3719-84-4
IT
                1874-47-1
                             2491-91-0
                                          3558-65-4
     835-71-2
                                                          16107-85-0
                  7753-06-2
                              10127-84-1
                                            14117-13-6
     6726-45-0
                   16107-88-3 16107-90-7
                                            16107-91-8
     16107-87-2
     16112-12-2
                  16112-14-4
                                16112-16-6
                                              16112-17-7
                                                            16112-21-3
                                              16112-27-9
                                                            16112-32-6
     16112-22-4
                   16112-24-6
                                16112-26-8
                                                            16112-37-1
                  16112-34-8
                                16112-35-9
                                              16112-36-0
     16112-33-7
                                              16112-41-7
                                                            16112-42-8
     16112-38-2
                   16112-39-3
                                16112-40-6
                                16151-03-4
                                              16151-04-5
                                                            16151-05-6
     16112-43-9
                   16112-44-0
                   16151-08-9
                                16151-77-2
                                              16155-54-7
                                                            16155-55-8
     16151-06-7
                                16155-59-2
                                              16155-60-5
                                                            16155-94-5
                   16155-58-1
     16155-57-0
                                              16155-98-9
                                                            16156-00-6
     16155-95-6
                   16155-96-7
                                16155-97-8
                                              22105-80-2
                                                            51390-15-9
                                16156-03-9
     16156-01-7
                   16156-02-8
     51390-16-0
        (reaction of, with benzylideneaniline derivs. in the presence of
        base)
```

L18 ANSWER 17 OF 27 HCA COPYRIGHT 2003 ACS 80:49274 Fluorescent whiteners. Siegrist, Adolf E.; Liechti,

Peter; Maeder, Erwin; Meyer, Hans Rudolf (Ciba-Geigy A.-G.).
Patentschrift (Switz.) CH 539101 19730831, 21 pp. (German). CODEN:
SWXXAS. APPLICATION: CH 1966-13743 19660923.

Twenty-five fluorescent whiteners [I, R, R1 = H, CMe3, Ph, Me, p-MeOC6H4CH:CH, p-ClC6H4CH:CH, PhCH:CH, p-PhC6H4CH:CH; R2 = H,Me; R3 = H, Cl, MeO, CO2Et, Ph; (R3R4) = benzo; (R4,R5) = benzo; R4,R5 = H; X, Y = CH, N] were prepd. and were incorporated into polyester and polyamide melts to give fibers having good whiteness. Thus, 2,4-diphenyl-6-p-tolyl-s-triazine was heated with p-MeOC6H4CH:NPh in DMF in the presence of KOCMe3 to give fluorescent whitener I(R = R1 = R2 = R4 = R5 = H; R3 = MeO, X = Y = N) [16155-78-5].

IT 16155-78-5P 16155-79-6P 16155-80-9P 16155-81-0P 16155-82-1P 16155-83-2P 16155-84-3P 16155-85-4P 16155-86-5P 16155-87-6P 16155-88-7P 16155-89-8P 16476-98-5P 36498-04-1P 42944-07-0P

(prepn. of)

RN 16155-78-5 HCA

CN 1,3,5-Triazine, 2-[4-[2-(4-methoxyphenyl)ethenyl]phenyl]-4,6-diphenyl- (9CI) (CA INDEX NAME)

$$CH = CH - N N N$$
MeO

RN 16155-79-6 HCA

CN 1,3,5-Triazine, 2-[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 16155-80-9 HCA

CN 1,3,5-Triazine, 2-phenyl-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-81-0 HCA

CN 1,3,5-Triazine, 2-[4-(1,1-dimethylethyl)phenyl]-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-82-1 HCA

CN 1,3,5-Triazine, 2-[1,1'-biphenyl]-4-yl-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-83-2 HCA

CN 1,3,5-Triazine, 2,4-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-6-phenyl- (9CI) (CA INDEX NAME)

RN 16155-84-3 HCA

CN 1,3,5-Triazine, 2,4-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-6-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-85-4 HCA

CN 1,3,5-Triazine, 2-[1,1'-biphenyl]-4-yl-4,6-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-86-5 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-87-6 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-(9CI) (CA INDEX NAME)

RN 16155-88-7 HCA

CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(4-chlorophenyl)ethenyl]phenyl](9CI) (CA INDEX NAME)

RN 16155-89-8 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(4-methoxyphenyl)ethenyl]phenyl]-(9CI) (CA INDEX NAME)

RN 16476-98-5 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-(2-[1,1'-biphenyl]-4-ylethenyl)-2methylphenyl]- (9CI) (CA INDEX NAME)

RN 36498-04-1 HCA CN Benzoic acid, 4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 42944-07-0 HCA CN 1,3,5-Triazine, 2,4-bis(4-methylphenyl)-6-[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

(prepn. of)

IC C08K; C11D CC 40-11 (Dyes, Fluorescent Whitening Agents, and Photosensitizers) ST stilbene fluorescence whitener; triazine fluorescent whitener; pyrimidine fluorescent whitener; pyridine fluorescent whitener Polyamide fibers IT Polyester fibers (fluorescence brighteners for, triazinyl stilbene derivs. as) Fluorescent brighteners IT (triazinylstilbene derivs., for polyamide and polyester fibers) 16155-78-5P 16155-79-6P 16155-80-9P IT 16155-81-0P 16155-82-1P 16155-83-2P 16155-84-3P 16155-85-4P 16155-86-5P 16155-87-6P 16155-88-7P 16155-89-8P 16184-21-7P 16184-22-8P 16184-24-0P 16184-25-1P 16184-26-2P 16325-04-5P 16263-29-9P 16263-30-2P 16263-16-4P 16476-98-5P 36498-04-1P 42944-00-3P 42944-07-0P

L18 ANSWER 18 OF 27 HCA COPYRIGHT 2003 ACS
76:128838 Benzoxazole derivatives for use as **fluorescent**whiteners. Meyer, Hans Rudolf; Siegrist, Adolf E. (Ciba-Geigy A.-G.). Ger. Offen. DE 2129816 19711230, 49 pp. (German). CODEN:
GWXXBX. APPLICATION: DE 1971-2129816 19710616.

Ten title compds. (I, R = H, Cl, Me, iso-Pr, tert-Bu, CMe2Ph, Ph, CMe2CH2CMe3, cyclohexyl; R1 = H, Me), useful for whitening polyesters, polyamides, poly(vinyl chloride), polystyrene, and cellulose acetate, were prepd. by condensing 4'-(2-benzoxazolyl)-4-stilbenecarbonyl chlorides with p-R1C6H4CN, in the presence of Friedel-Crafts catalysts, cooling, and adding NH3 or by condensing a 4'-(triazinyl)-4-stilbenecarboxylic acid (or the acid chloride or ester deriv.) with an o-aminophenol followed by ring closure. For example, 4'-(5-tert-butyl-2-benzoxazolyl)-4-stilbenecarboxylic acid was treated with SOCl2, the acid chloride treated with PhCN, SOCl2, and AlCl3 at 130.deg., cooled to 80.deg., dild. with CCl4 and NH3 added to give bright yellow 4-(5-tert-butyl-2-benzoxazolyl)-4'-(4,6-

triazin-2-yl)phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 36498-03-0 HCA CN Benzoxazole, 2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]-5-methyl- (9CI) (CA INDEX NAME)

RN 36498-04-1 HCA CN Benzoic acid, 4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 36498-05-2 HCA

CN Benzoic acid, 4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 36498-06-3 HCA

CN Benzoyl chloride, 4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 36498-07-4 HCA

CN Benzoic acid, 4-[2-[4-[4,6-bis(4-methylphenyl)-1,3,5-triazin-2-yl]phenyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 36498-08-5 HCA

CN Benzoic acid, 4-[2-[4-[4,6-bis(4-methylphenyl)-1,3,5-triazin-2-yl]phenyl]- (9CI) (CA INDEX NAME)

RN 36498-09-6 HCA

CN Benzoxazole, 2-[4-[2-[4-[4,6-bis(4-methylphenyl)-1,3,5-triazin-2-yl]phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 36536-07-9 HCA

CN Benzoxazole, 2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-

yl)phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 36536-08-0 HCA

CN Benzoxazole, 5-chloro-2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]- (9CI) (CA INDEX NAME)

RN 36565-19-2 HCA

CN Benzoxazole, 2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]-5-(1-methylethyl)- (9CI) (CA INDEX NAME)

RN 36576-58-6 HCA

CN Benzoxazole, 2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]-5-(1-methyl-1-phenylethyl)- (9CI) (CA INDEX NAME)

RN 36576-59-7 HCA

CN Benzoxazole, 2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]phenyl]-5-phenyl- (9CI) (CA INDEX NAME)

RN 36576-60-0 HCA

CN Benzoxazole, 5-cyclohexyl-2-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]- (9CI) (CA INDEX NAME)

RN 36576-61-1 HCA

CN Benzoxazole, 2-[4-[2-[4-(4,6-diphenyl-1,3,5-triazin-2-yl)phenyl]ethenyl]-5-(1,1,3,3-tetramethylbutyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{Me} \\ \text{Me} \\ \text{Me} \end{array}$$

IC C07D

CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers) Section cross-reference(s): 28

melt spinning fluorescent whitener; fluorescent
whitener benzoxazolylstilbene; triazinylstilbene fluorescent
whitener; polyester fluorescent whitener; polyamide
fluorescent whitener; polystyrene fluorescent
whitener; PVC fluorescent whitener; cellulose acetate
fluorescent whitener; stilbene fluorescent
whitener

IT Fluorescent brighteners

(benzoxazolyl stilbene derivs., for synthetic fibers and polymers)

IT Polyamide fibers

Polyester fibers

(fluorescent brighteners for, benzoxazolyl stilbene derivs. as)

IT 9002-86-2 9003-53-6

(fluorescent brighteners for, benzoxazolyl stilbene derivs. as)

IT 5017-62-9P 34599-17-2P 36498-03-0P

36498-04-1P 36498-05-2P 36498-06-3P

36498-07-4P 36498-08-5P 36498-09-6P

36536-07-9P 36536-08-0P 36565-19-2P

36576-58-6P 36576-59-7P 36576-60-0P

36576-61-1P

(prepn. of)

L18 ANSWER 19 OF 27 HCA COPYRIGHT 2003 ACS

76:101063 Comparison of **fluorescent** brightening in the production of synthetic-polymer fibers and in the textile industry. Eckhardt, C.; Hefti, H. (Ciba-Geigy Ltd., Basel, Switz.). Journal of the Society of Dyers and Colourists, 87(11), 365-70 (English) 1971. CODEN: JSDCAA. ISSN: 0037-9859.

AB Methods for mass whitening of synthetic polymer fibers are briefly reviewed and the chem. and phys. characteristics of **fluorescent** whiteners for polyester and nylon fibers, both

for addn. in the mass and for conventional application during textile processing, are discussed. The whitening and fastness effects obtained on polyester by benzoxazolylethylene deriv. I and benzoxazolylstilbene deriv. II applied by the pad-thermofix process were comparable to those obtained with the triazinylstilbene deriv. III incorporated before extrusion. On both textile application and mass whitening, conventional diaminostilbenedisulfonic acid derivs. showed poorer fastness properties than the newer distyryl biphenyl deriv. IV. The **fluorescent** whiteners did not affect the dyeing behavior of mass-whitened nylon. Methods for distinguishing between textile-and mass-whitening effects are discussed.

IT 6888-33-1

(polyester fibers optically brightened by, effect of application method and concn. and exposure time on)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

CC 39 (Textiles)

ST fluorescent whitening polyester; nylon fluorescent whitening

IT Polyamide fibers

Polyester fibers

Synthetic fibers

(fluorescent brighteners for, conventional application and mass brightening in relation to)

IT Fluorescent brighteners

(for synthetic fibers, by conventional application and mass brightening)

IT 6888-33-1

(polyester fibers optically brightened by, effect of application method and concn. and exposure time on)

L18 ANSWER 20 OF 27 HCA COPYRIGHT 2003 ACS

76:47391 P,P'-Bis(benzoxazolyl)tolan derivatives. Meyer, Hans Rudolf; Liechti, Peter; Weber, Kurt; Siegrist, Adolf E. (CIBA Ltd.). U.S. US 3609160 19710928, 9 pp. (English). CODEN: USXXAM. APPLICATION: US 1967-659343 19670809.

AB Tolan derivs., useful as **fluorescent** whiteners for cotton or polyesters, were prepd. For example, 0.01 mole p,p'-tolandicarboxylic acid dichloride was heated with 0.02 mole 2-amino-3-hydroxybiphenyl in chlorobenzene to give the amide I. I was then dried and heated under N in a salt bath to give

p,p'-bis(5-phenylbenzoxazol-2-yl)tolan (II) [25851-07-4]. Nine other sym. and unsym. compds. contg. heterocyclic para substituents were prepd.

IT 25739-16-6P 25739-17-7P

(prepn. of)

RN 25739-16-6 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethynediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 25739-17-7 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethynediyldi-4,1-phenylene)bis[4,6-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

IC CO7D; CO1D

NCL 260307000D

CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
Section cross-reference(s): 25, 28

ST tolan polyester whitener; **fluorescent** whitener tolan; textile whitener tolan

IT Fluorescent brighteners

(tolan derivs.)

IT 16819-44-6P 24170-42-1P 24170-43-2P 25739-11-1P 16819-43-5P 25739-13-3P **25739-16-6P 25739-17-7P** 25739-12-2P 25739-20-2P 25739-21-3P 25739-22-4P 25739-18-8P 25739-19-9P 25739-26-8P 25739-27-9P 25739-25-7P 25739-23-5P 25739-24-6P 25739-32-6P 25739-28-0P 25739-29-1P 25739-30-4P 25739-31-5P 25851-10-9P 25851-08-5P 25851-09-6P 25739-33-7P 25851-07-4P

35101-13-4P (prepn. of)

L18 ANSWER 21 OF 27 HCA COPYRIGHT 2003 ACS
73:67750 Inorganic white pigments containing fluorescent
whitening agents. Preininger, Erich; Ging, Dieter (CIBA, Ltd.).
Ger. Offen. DE 1959233 19700618, 56 pp. (German). CODEN: GWXXBX.
APPLICATION: DE 1969-1959233 19691126.

AB Inorg. pigments are slurried in H2O with 0.1-15% (based on wt. of the pigment) of **fluorescent** whiteners having soly. <0.5 parts/100 H2O, one or more nonionic surfactants, and other adjuvants or coating agents. Upon sepn. of the solids from the slurry, washing and drying, the whiteners and other additives are deposited on the pigment surfaces.

IT 6888-33-1

(titanium oxide pigments coated with, fluorescent)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

IC C09C

CC 42 (Coatings, Inks, and Related Products)

IT Nylon, uses and miscellaneous

(coatings, contq. fluorescent white pigments)

IT Coating materials

(fluorescent dyes, on white pigments)

IT Pigments

(titanium oxide, **fluorescent** whitening agents-coated)

IT 1314-98-3, uses and miscellaneous

(coatings on, of **fluorescent** whitening agents)

IT 9002-86-2, uses and miscellaneous 9002-88-4, uses and miscellaneous 9003-56-9, uses and miscellaneous (coatings, contq. **fluorescent** white pigments)

IT 2397-00-4 4751-43-3 6394-12-3 **6888-33-1** 7128-64-5 13468-27-4 28865-48-7 28865-49-8 (titanium oxide pigments coated with, **fluorescent**)

L18 ANSWER 22 OF 27 HCA COPYRIGHT 2003 ACS

72:134172 4,4'-Bistriazinylstilbenes. Siegrist, Adolf E.; Maeder, Erwin; Liechti, Peter; Guglielmetti, Leonardo (CIBA Ltd.). Patentsc hrift (Switz.) CH 479598 19691128, 6 pp. (German). CODEN: SWXXAS. APPLICATION: CH 1964-479598 19640923.

GI For diagram(s), see printed CA Issue.

The title compds. (I), prepd. by heating p-ClCOC6H4CH:CHC6H4COCl-p (II) with 4 moles p-RC6H4CN in the presence of anhyd. AlCl3 and heating the intermediate product with NH4Cl, exhibit fluorescence, good stability to heat, light, and migration, and are suitable in amts. of 0.01-0.2% as brighteners for various natural or synthetic org. materials. Thus, 14.46 g II and 30.9 g PhCN were stirred in 200 ml dry o-C6H4Cl2, treated with 13.3 g anhyd. AlCl3, heated to 120.degree., treated with 10.6 g NH4Cl, and stirred at 120.degree. for 15 hr to yield 24 g I (R = H), m. g390.degree. (o-C6H4Cl2). Similarly was prepd. I (R = Me), m. 374-6.degree.

IT 6568-89-4P 6888-33-1P

(prepn. of)

RN 6568-89-4 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

IC CO7D

CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

IT Fluorescent brightening agents

((vinylenedi-p-phenylene)bis[diphenyltriazine] derivs.)

IT 6568-89-4P 6888-33-1P

(prepn. of)

L18 ANSWER 23 OF 27 HCA COPYRIGHT 2003 ACS 72:56714 Tolan **fluorescent** whitening agents. (Ciba Ltd.). Fr

FR 1547502 19681129, 15 pp. (French). CODEN: FRXXAK. PRIORITY: CH 19660815.

GI For diagram(s), see printed CA Issue.

AΒ

The title compds. have the general formula I, where Y1 and (or) Y2 are heterocyclic residues. Thus, a mixt. of 3.03 g I (Y1 = Y2 = COC1, R = H) (II), 2.18 g 2 -HOC6H4NH2, and 80 ml PhCl was heated during 30 min to 115.degree. with a gitation by a stream of N, and held at 115.degree. for 19 hr to give 4.5 g I (Y1 = Y2 = 2-HOC6H4NHCO, R = H), which was heated dry in N on a salt bath at 325.degree. (melted and resolidified with sepn. of H2O), and heated for 15 min at 350.degree. to give 4.0 g I (R = H, Y1 = Y2 = Z1) (III) (R1 = R2 = H), yellowish white crystals, m. 360-2.degree. (HCONMePh, C6H3Cl3). Similarly, other III were prepd. [R1, R2, and m.p. (C6H3Cl3) given]: Me3C, H, 294-6.degree.; Ph, H, 343-5.degree.; H, Ph, 356-8.degree.. A mixt. of 3.03 g II, 12.4 g PhCN, and 3.03 g 88% AlCl3 was stirred for 1 hr at 115.degree., dild. with 40 ml CCl4, and NH3 added during 1.25 hr under reflux (76.degree.) until the mixt. was decolorized to give 5.5 g I (R = H, Y1 = Y2 = Z2) (IV) (R' = H), m. 390-90.5.degree. (o-C6H4Cl2). Similarly was prepd. IV (R' = Me), m. 372.5-3.degree. (o-C6H4Cl2). II and 2-02NC6H4NH2 gave I (R = H, Y1 = Y2 = 2-02NC6H4NHCO), m. 264-7.degree., which with SnCl2 gave I [R = H, Y1 = Y2 = 2-benzimidazolyl (Z3)], m. >360.degree. I (R = Y1 = H, Y2 = COCl) and 2,4-HO(Ph)C6H3NH2 gave I [R = Y1 = H, Y2 = 2,4-HO(Ph)C6H4NHCO], m. 251-3.degree., which with B2 o3 gaveI [R = Y1 = H, Y2 = Z1 (R1 = H, R2 = Ph), m. 196-8.degree. (o-C6H4Cl2). Similarly were prepd. other I (R = Y1 = H) (Y2 and m.p. given): 2-O2NC6H4NHCO,142-4.degree.; Z3, 287-8.degree.; and I [R = H, Y1 = Ph, Y2 = Z1(R1)]= H, R2 = Ph)], m. 248-9.degree. (dioxane), I (Y1 = Y2 = NH2, R = SO3H) was tetrazotized and coupled with 2,5-H2NC10H6SO3H, the bi s-o-aminoazo compd. treated with concd. aq. NH3 and CuSO4 to give I (R = SO3Na, Y1 = Y2 = Z4) (V) (R1 = SO3Na, R2 = R3 = H). Similarly, other V were prepd. (R1-R3 given): H, H, H; H, SO3Na, H; H, H, SO3Na; SO3Na, H, SO3Na. Also prepd. were I (Y1 = Y2 = Z5, R = V2)SO3Na), I (Y1 = Y2 = 5-methoxy-6-methyl-2-benzotriazolyl, R = SO3Na), and I [R = H, Y1 = Y2 = Z4 (R1 = R3 = H, R2 = SO3Na)]. Prepn. of intermediates: A soln. of 486 q 4-EtO2C-C6H4CH:CHC6H4CO2Et - 4 in 4.5 l. CHCl3 was treated during 2.5 hr with 262 g Br, and stirred overnight at room temp. to give 400 g 4-EtO2CC6H4CHBrC6H4CO2Et - 4, m. 192-4.degree., which (484 g) was dissolved in 4 l. BuOH and 1.25 kg KOH (contg. 10% H2O), refluxed at 125.degree. with stirring for 3 hr, dild. with 8 l. H2O, BuOH steam-distd., and the aq. phase acidified to Congo red with HCl to give 255 g I (Y1 = Y2 = CO2H, R = H) (VI), m. >360.degree.. A mixt. of 213 g VI, 2 l. PhCl, and 1 ml HCONMe2 was treated at 105.degree. during 70 min with 180 ml SOCl2, stirred for 10 min, and evapd. under vacuum to dryness to give 207 g II, m. 148-50.degree. (C2Cl4). 4-PhCH:CHC6H4CO2Me was brominated to 4-PhCHBrCHBrC6H4CO2Me, m. 196-8.degree., which was treated with KOH in BuOH to give 4-PhC.tplbond.CC6H4CO2H, m. 208-10.degree. (sublimed in vacuo, m. 220-30.degree.), which with SOCl2 gave 4-PhC.tplbond.CC6H4COCl, m. 89-90.degree. (CHCl3); similarly, 4-PhC6H4CH:CHC6H4CO2Me, m.

232-4.degree. gave the dibromo compd., m. 216-18.degree.; from which was prepd. I (R = H, Y1 = Ph, Y2 = CO2H), m. 291.degree..

IT 25739-16-6P 25739-17-7P

(prepn. of)

RN 25739-16-6 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethynediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 25739-17-7 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethynediyldi-4,1-phenylene)bis[4,6-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

IC C07D; C09B

CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

IT Fiber, polyester, uses and miscellaneous

(fluorescent brightening agents for, heterocyclic tolan derivs. as)

IT Fluorescent brightening agents

(heterocyclic tolan derivs., for polyester fibers)

24170-42-1P 25739-11-1P 25739-12-2P IT 16819-43-5P 16819-44-6P 25739-13-3P 25739-16-6P 25739-17-7P 25739-20-2P 25739-21-3P 25739-22-4P 25739-18-8P 25739-19-9P 25739-26-8P 25739-27-9P 25739-24-6P 25739-25-7P 25739-23-5P 25739-32-6P 25739-28-0P 25739-29-1P 25739-30-4P 25739-31-5P 25739-33-7P 25739-34-8P 25851-07-4P 25851-08-5P 25851-09-6P 25851-10-9P

(prepn. of)

L18 ANSWER 24 OF 27 HCA COPYRIGHT 2003 ACS

71:126002 4,4'-Bis-triazinyl stilbenes. Siegrist, Adolf E.; Maeder, Erwin; Liechti, Peter; Guglielmetti, Leonardo (CIBA Ltd.). Patentschrift (Switz.) CH 472416 19690630, 7 pp. (German). CODEN: SWXXAS. APPLICATION: CH 1965-472416 19650722.

GI For diagram(s), see printed CA Issue.

AB Compds. of the formula I useful as **fluorescent** whitening agents for natural and synthetic fibers were prepd. Thus, 13.3 parts dry AlCl3 was added to a mixt. of 14.46 parts (4-ClCOC6H4CH:)2 30.9 parts PhCN, and 200 parts dry o-C6H4Cl2, heated to 120.degree., treated with 10.6 parts NH4Cl, stirred at 120.degree. for 15 hrs., cooled, and poured into H2O, to give 24 parts I (R = H), light yellow needles, m. >390.degree.. Similarly, the following yellow I were prepd.: (R, % yield, and m.p. given): 4-Me, 87.4, 374-6.degree.; 4-tert-Bu, 80.4, >420.degree.; 4-MeO, 85.5, 306-7.degree.; 4-Cl, 82.5, 373-4.degree.; 3-Cl, 81.1, 385-6.degree..

IT 6568-89-4P 6568-90-7P 6568-91-8P 6739-71-5P 6888-33-1P 6888-34-2P

(prepn. of)

RN 6568-89-4 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)

RN 6568-90-7 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(p-tert-butylphenyl)- (7CI, 8CI) (CA INDEX NAME)

RN 6568-91-8 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(m-chlorophenyl)-(7CI, 8CI) (CA INDEX NAME)

RN 6739-71-5 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(p-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 6888-34-2 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(p-chlorophenyl)-(7CI, 8CI) (CA INDEX NAME)

IC C07D

CC 40 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)

ST triazinyl stilbenes fluorescent whiteners;

fluorescent whiteners triazinyl stilbenes; stilbenes

triazinyl fluorescent whiteners; whiteners

fluorescent triazinyl stilbenes

IT **Fluorescent** brightening agents

((vinylenediphenylene)bis(diphenyltriazine) derivs.)

IT 6568-89-4P 6568-90-7P 6568-91-8P

6739-71-5P 6888-33-1P 6888-34-2P

(prepn. of)

L18 ANSWER 25 OF 27 HCA COPYRIGHT 2003 ACS

70:38906 Heterocyclic stilbenes. (CIBA Ltd.). Fr. FR 1506629 19671222,

12 pp. (French). CODEN: FRXXAK. PRIORITY: CH 19651202.

GI For diagram(s), see printed CA Issue.

The title compds., as **fluorescent** whitening agents for incorporation in polyester fibers, were prepd. by aerating the corresponding p-tolyl heterocyclic compds. in HCONMe2 in the presence of KOH. Thus, dry air (1-3 1./hr.) was passed for 15-18 hrs. through a mixt. contg. 20.9 g. 2-p-tolylbenzoxazole (I), 12.5 g. KOH powder contg. 10% H2O, and 250 ml. HCONMe2, the mixt. heated at 50-60.degree. until it became yellowish brown, and treated with 500 ml. MeOH to give 11.2 g. (54%) 4,4'-bis(2-benzoxazolyl)stilbene (II, R = H), greenish-yellow needles m. 362-3.degree. (o-C6H4Cl2).

Similarly prepd. in 33% yield was II (R = tert-Bu), m. 320-20.5.degree. (C2Cl4), from the 5-tert-Bu deriv. of I. The following III were similarly prepd. (Ar, X, % yield, and m.p. given): 4-tert-BuC6H4, O, 43, 350.0-50.5.degree. (.omicron.-C6H4Cl2); 4-MeOC6H4, O, 25, 293.5-4.5.degree.; 2-thienyl, S, 17, 346.5-7.5.degree.. The following IV were similarly prepd. (X, Y, % yield, and m.p. given): N, CPh, 19, 348.0-8.5.degree.; CPh, N, 41, 357-60.degree.. 4,4'-Bis(4-phenyl-2-quinazolinyl)stilbene, 54% yield, m. 335-5.5.degree.; 4,4'-bis(2-benzotriazolyl)stilbene, 20% yield, m. 377.5-8.5.degree.; and 4,4'-bis(4,5-diphenyl-2-oxazolyl)stilbene, 25% yield, m. 292.degree. (xylene), were also prepd.

IT 6888-33-1P

(prepn. of)

RN 6888-33-1 HCA

CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

IC C07D; C09B

CC 40 (Dyes, Fluorescent Brightening Agents, and Photosensitizers)

ST stilbenes; optical brighteners; brighteners optical; whiteners fluorescent; benzoxazoles; oxadiazoles; triazines

IT Fluorescent brightening agents

(stilbene derivs. of heterocycles)

IT 1533-45-5P 2397-01-5P 6394-10-1P 6394-12-3P **6888-33-1P**14317-94-3P 19530-52-0P 19551-18-9P 19551-19-0P 20982-05-2P
(prepn. of)

L18 ANSWER 26 OF 27 HCA COPYRIGHT 2003 ACS

68:21961 Alkenic unsaturated heterocyclic compounds. (CIBA Ltd.). Neth. Appl. NL 6615211 19670502, 138 pp. (Dutch). CODEN: NAXXAN. PRIORITY: CH 19651028 - 19660704 19660704.

GI For diagram(s), see printed CA Issue.

The title compds. are prepd. by treating compds. of the general formula I with a Schiff base in the presence of a strongly basic alkali metal compd. in a polar, neutral to alk., solvent, which is free of atoms replaceable by alkali metal and practically free of H2O. I contains R1 which is a heterocyclic ring system of aromatic nature contg. .gtoreq.1 heterocyclic 5- or 6-ring with .gtoreq.1 N ring atom and which is free of H atoms bound to the N ring atom and bound with a part of the ring to a part of the ring R2 or contains 2 vicinal ring parts in common with 2 vicinal ring parts of R2, and contains a part R2 which is a carbocyclic or heterocyclic ring

system of aromatic nature contg. a 5- or 6-ring and possibly more condensed aromatic or hydroaromatic ring systems; Me in I is in the para position with respect to the R1 bond. If the reaction takes place in the presence of alkali metal hydroxides, the H2O content should be <25%. The following codes are used throughout the abstract: Radicals (rings are always substituted at the para position) are indicated as follows: A = CH:CHPh, A1 = CH:CHC6H4Ph, A2 = CH:CHC6H4C1, A3 = CH:CHC6H4OMe, A4 = 1-C10H7CH:CH, A5 =2-C10H7CH:CH, B = C6H4CH:CHPh, B1 = C6H4CH:CHC6H4Ph, B2 =C6H4CH:CHC6H4Cl, B3 = C6H4CH:CHC6H4OMe, B4 = C6H4CH:CHC10H7-1, B5 = C6H4CH:CHC10H7-2, B6 = C6H4CH:CHC6H4CHMe2, C1 = C6H4Ph, C2 = C6H4Cl, C3 = C6H4OMe, C4 = C6H4CMe3, C5 = C6H4CHMe2, D1 = C6H4C6H4CH: CHPhand recrystn. solvents indicated as follows: 1 = H2O, 2 = EtOH, 3 = dioxane, 4 = dimethylformamide, 5 = tetrachloroethene, 6 = PhCl, 7 = o-dichlorobenzene, 8 = trichlorobenzene, 9 = toluene, 10 = n-hexane, 11 = xylene. Thus, 8.63 g. II (X = p-MeC6H4) and 7.05 g. 4'-methoxybenzalaniline were stirred in 200 ml. anhyd. dimethylformamide with exclusion of air, 11.2 g. K tert-butanolate was added in one step, the mixt. stirred 15 min., 400 ml. H2O added dropwise at 5-15.degree., the product sepd., washed with H2O to neutral and dissolved in 270 ml. dimethylformamide with heating, 25 ml. 10% HCl added, 300 ml. H2O added after a few min. and the mixt. cooled to .apprx.10.degree. to yield 93% II (X = B3), m. 214-14.5.degree. (tetrachloroethene). The same reaction but with 6.05 q. benzalaniline yielded 90% II (X = B), m. 173.5-74.degree. Similarly were prepd. the following benzoxazole derivs. (X1, X2, X3, % yield, and incor. m.p. given): 2-Ph, H, B, 57.7, 226-6.5.degree. (5); 2-Ph, H, B3, 61.6, 250-1.degree. (5); H, SO2NH(CH2)7Me, B, 66.2, 194-4.5.degree. (2); A, H, C1, 67.5, 203-3.5.degree. (5); A, H, Ph, 77.6, 146-6.5.degree. (2); A, H, C4, 77.3, 141-1.5.degree. (2); A3, H, C1, 60.5, 232-2.5.degree. (2/3); A3, H, C2, 51.4, 199-9.5.degree. (5); A1, H, Ph, 97.0, 215-16.degree. (5); A1, H, C4, 92.1, 199.5-200.degree. (5); A1, H, C1, 87.5, 289-9.5.degree. (6); A5, H, C4, 100, 185.5-86.degree. (2/3); A5, H, C1, 76.7, 248-9.degree. (5); A, Me, C1, 74.4, 179.5-80.5.degree. (2/3); A1, Me, C1, 100, 259-9.5.degree. (4); A5, Me, C1, 78.6, 228-8.5.degree. (2/3); A4, Me, C1, 85.0, 202.5-203.degree. (2/3); A2, Me, C1, 66.4, 200-1.degree. (2); A3, Me, C1, 52.6, 191.5-92.degree. (10/11); A, Me, B, 43.5, 222.3.degree. (2/3); A1, Me, B, 90.5, 296.5-8.5.degree. (7); A, H, B, 22, 260-60.5.degree. (5); the following quinazoline derivs. of formula IV (X1, X2, X3, and X4, % yield, and m.p. given): H, H, Ph, B1, 94.3, 226.5-27.degree. (5); A, H, Ph, Ph, 93.5, 198-8.5.degree. (5); A1, H, Ph, Ph, 97.0, 243-3.5.degree. (2/3); A1, H, Ph, B1, 96.5, 384-5.degree. (7); H, A, Ph, Ph, 87.5, 166-6.5.degree. (2/3); H, A1, Ph, Ph, 92.5, 242-2.5.degree. (5); H, H, B, Ph, 92.0, 218-19.degree. (5); H, H, B1, Ph, 97.7, 300-1.degree. (7); the following compds. V (X, X1 = X2, % yield, and m.p. given): S, B3, 83.5, 300-300.5.degree. (7); O, B3, 89, 311-11.5 (7); the following 1,2,4-oxadiazole derivs. VI (X1, X2, % yield, and m.p. given): B, Ph, 70.2, 159-9.5.degree. (1); B1, Ph, 75.0, 228-8.5.degree. (5); B, B, 64.2, 246-7.degree. (5); B1, B1, 91.7, 329-30.degree. (6); the

following 1,3,5-triazine derivs. VII (X1, X2, X3, % yield, and m.p. given): Ph, B3, Ph, 100, 235.5.degree. (2/3); B, B, B, 99.5, 275-7.degree. (5); B3, B3, B3, 96.6, 300.degree. (5); B1, B1, B1, 93.1, 361-2.degree. (7); B2, B2, B2, 94.0, 315-17.degree. (5); Ph, B1, Ph, 98.5, 284-5.degree. (5); B1, o-Me-B1, o-Me-B1, 100, 162-2.5.degree. (11); B, B, Ph, 96.6, 241-1.5.degree. (5); B, B, C4, 97.0, 230.5-31.degree. (9/10); B, B, C1, 94.3, 240.5-41.degree. (5); B1, B1, Ph, 94.9, 351-2.5.degree. (9); B1, B1, C4, 98.0, 325-8.degree. (2/3); B1, B1, C1, 91.7, 359-60.degree. (7); the following compds. VIII (X1, X2, X3, % yield, and m.p. given): 2-Ph, 2-Ph, B, 69.2, 202.5-3.5.degree. (4/2/1); 2-Ph, 2-Ph, B1, 85.5, 264-5.degree. (4). A mixt. of II (X = p-MeC6H4) (12.96 g.), 9.1 g. benzalaniline and 25 g. KOH powder with .apprx.10% H2O in 300 ml. dimethylformamide was stirred, heated to 60.degree. in 30 min., stirred 30 min. at 60.degree., cooled to room temp., 100 ml. H2O and 240 ml. 10% HCl added dropwise, the product washed with H2O and 80 ml. MeOH and dried to yield .apprx.15.7 g. (90.5%) II (X = B), m. 182-2.5.degree. (5). Similarly were prepd. the following naphthotriazole derivs. II (X, % yield, and m.p. given): B1, 91.2, 215-15.5.degree. (5); B2, 86.2, 237.5-38.degree. (5); B1, 92.6, 255-6.degree. (7); B4, 94.6, 215-15.5.degree. (5); B5, 79.5, 236-7.degree. (5); C6H4CH:CHCl-2-C6H4, 66.0, 182-82.5.degree. (5); C6H11CH: CHC6H4CHMe2, 84.4, 173.5-74.degree. (2/4); 3,4-methylenedioxyphenyl, 69.5, 232-3.degree. (5); the following benzotriazole compds. IX (X, % yield, and m.p. given): B, 49.8, 196-96.5.degree. (2); B1, 86.7, 271-71.5.degree. (5); the following 1,3,4-oxadiazole derivs. V (X = 0) (X1, X2, % yield, and m.p.given): C1, B3, 68.3, 248-8.5.degree. (5); Ph, B, 50.6, 168.5-9.5.degree. (2); C4, B, 59.4, 166-7.degree. (2); C1, B, 72.5, 227-8.degree. (5); B, B, 84.9, 278-9.degree. (7); D1, B, 85.6, 309-10.degree. (7); Ph, B1, 84.0, 217-17.5.degree. (5); C4, B1, 88.4, 235-5.5.degree. (5); C1, B1, 88.5, 286.5-87.degree. (7); B, B1, 90.9, 305-6.degree. (7); B1, B1, 93.6, 371-2.5.degree. (8); D1, B1, 86.5, 375-6.degree. (7); Ph, B2, 64.0, 209.5-10.degree. (5); C4, B2, 67.0, 217.5-19.degree. (5); C1, B2, 78.4, 250-1.degree. (7); B, B2, 73.8, 289-90.degree. (5); B2, B2, 88.2, 310-11.degree. (7); Ph, B3, 58.1, 176.degree. (5); C4, B3, 65.7, 190.5-91.degree. (5); B3, B3, 83.0, 310-11.degree. (7); Ph, B4, 85.4, 188.5-9.5.degree. (5); C4, B4, 71.5, 164.5-5.5.degree. (5); Ph, B5, 66.3, 200.5-202.degree. (7); C4, B5, 69.9, 219-19.5.degree. (5); C1, B5, 71.0, 265-5.5.degree. (7); C1, B4, 79.0, 218.5-19.degree. (2/4). of V (X = 0, X1 = X2 = p-MeC6H4) 12.52 g., 12.52 g. benzalalanine, 12.6 g. KOH powder contg. .apprx.10% H2O and 300 ml. dimethylformamide was stirred, the temp. of the mixt. increased to 90.degree. over 25 min., the mixt. stirred 40 min. at 90-5.degree., cooled to 10.degree.; 100 ml. H2O and 140 ml. 10% HCl and 250 ml. H2O added dropwise at 10-20.degree. and the product worked up to yield 84.5% 2,5-bis(stilben-4-yl-1,3,4-oxadiazole, m. 279-80.degree. Similarly prepd. were the following 1,3,4-oxadiazoles and 1,3,4-thiadiazoles, V (X1 = X2) (X, X1, % yield, m.p., and reaction temp. given): O, B2, 96, 305-5.5.degree. (7), 90-5.degree.; O, B3, 75.2, 309.5-10.degree. (7), 90-5.degree.; O, B5, 92.0, 334-5.degree.

(7), 60.degree.; S, B, 93.2, 361-2.degree. (7), 60.degree.; S, B1, 94.9, >400.degree. (8), 60.degree.; O, B6, 91.6, 285-86.5.degree. (11), 60.degree.; O, B4, 92.5, 255-5.5.degree. (11), 60.degree.. Also prepd. in the presence of KOH contq. 10% H2O were 53.2% III (X1 = 2-Ph, X2 = H, X3 = B), m. 224-4.5.degree. (5) and the following4-(aryloxazol-2-yl)stilbene derivs. III at a reaction temp. of 60.degree. and in the presence of 4 moles KOH/Me group (X1, X2, X3, % yield, and m.p. given): H, H, B, 45.7, 197-7.5.degree. (2); H, CMe3, B, 51.0, 174-4.5.degree. (2); H, Me, B, 43.4, 182.5-83.degree. (2); Me, H, B, 32.1, 180-80.5.degree. (1/4); H, 2-Ph, B, 55.2, 233-3.5.degree. (5); H, C(CH3)2Ph, B, 36.2, 144-4.5.degree. (2/3); Me, Me, B, 78.0, 233-3.5.degree. (5); H, H, B2, 69.4, 239-9.5.degree. (5); H, CMe3, B2, 71.7, 228.5-29.degree. (5); 2-Ph, H, B2, 58.7, 255-5.5.degree. (5); H, H, B3, 52.6, 220.5-22.degree. (2/3); H, CMe3, B3, 44.3, 211-11.5.degree. (5); H, CMe2Ph, B3, 53.9, 197-7.5.degree. (5); 2-Ph, H, B3, 56.6, 254-4.5.degree. (5); 2-Ph, H, B6, 72.5, 196.5-97.degree. (4); Me, Me, B, 78.0, 233-3.5.degree. (5); and the following corresponding naphthyl derivs. III (X1 = H) (X3, % yield, and m.p. given): B, 64.5, 204-4.5.degree. (2/3); B2, 75.5, 222-3.degree. (5); and B3, 56.2, 216-17.degree. (5). Reaction of 10.47 g. 1-(benzoxazol-2-yl)-4-methylbenzene, 12.87 g. biphenyl-4-carboxaldehyde anil and 25 g. KOH contg. 10% H2O in 300 ml. dimethylformamide and further workup gave 45.2% 4-(benzoxazol-2-yl)-4'-phenylstilbene m. 276-6.5.degree. (7). Similarly prepd. were the following 4-(aryloxazol-2-yl)-4'phenylstilbene derivs. III (X1, X2, % yield, and m.p. given) (X3 = B1): H, CMe3, 80, 264-5.degree. (4); H, CMe2Ph, 77.0, 238-8.5.degree. (5); H, 2-Ph, 69.0, 294.5-5.5.degree. (7); 2-Ph, H, 70.3, 284-4.5.degree. (7); H, Me, 77.6, 294.5-95.degree. (5); Me, H, 78.4, 280-80.5.degree. (4); Me, Me, 82.7, 306-8.degree. (5); H, SO2NH(CH2)7Me, 90, 266-6.5.degree. (5); and the 1-naphthyl deriv., 72.7, 259.5-60.degree. (7); the 2-naphthyl deriv., 94.8, 279-9.5.degree. (11); and compds. III (X3 = m-MeC6H4CH:CHC6H4Ph, X1 = X2 = H) 50.6, 213-213.5.degree. (5) and III (X3 = C)o-MeC6H4CH:CHC6H4Ph) 82.5, 201-2.degree. (5). Reaction of 5.23 g. III (X1 = X2 = H, X3 = p-MeC6H4) with 5.78 g. naphthalene-1carboxaldehyde anil in the presence of KOH in DMF and further workup as above yielded 89% III (X1 = X2 = H, X3 = B4), m. 165-6.degree. (2/3). Similarly prepd. were the following III (same data given): H, CMe3, B4, 89.4, 141-1.5.degree. (2/3); H, 2-Ph, B4, 90.0, 150.5-51.degree. (2/3); 2-Ph, H, B4, 95.8, 183-3.5.degree. (2/3); H, H, B5, 65.7, 225-6.degree. (2/3); H, CMe3, B5, 61.4, 208-8.5.degree. (2/3); H, 2-Ph, B5, 60.2, 261-1.5.degree. (7); 2-Ph, H, B5, 62.4, 264-5.degree. (5); H, H, o-MeC6H4CH:CHC10M7-1, 90, 144-4.5.degree. (2); H, H, m-MeC6H4CH:CHC10M7-1, 95.7, 168-8.5.degree. (5); and the following naphthyl derivs. (X3 given): B4, 72.5, 206.5-207.degree. (3); B5, 80.7, 256-6.5.degree. (5). Reaction of 10.42 g. bibenzoxazolyl (IIIa) with the bond at the X1 position, X2 = H, X3 = p-MeC6H4 (obtained by the condensation of 1 mole 3,3'-dihydroxybenzidine and 2 moles p-tolulic acid and subsequent heating to >200.degree. with boric acid as catalyst) with 9.06 g. benzalaniline and 25 g. KOH in 300 ml. dimethylformamide gave 75.6%

IIIa where the bond of III to III is at the X1 position, X2 = H and X3 = B, m. 352-3.degree. (7). Also prepd. was IIIa where X3 = B6 in 62.7% yield, m. >380.degree. (7). Other compds. prepd. were the 4-(benzthiazol-2-yl)stilbene derivs. X (X, % yield, and m.p. given): B, 80.6, 231-1.5.degree. (5); B2, 82.8, 263.5-64.degree. (5); B3, 90.8, 244.5-45.degree. (5); B1, 88.0, 299-300.degree. (7); B4, 92.5, 145.5-46.degree. (2/3); B5, 80.5, 249.5-50 (5); the 2-(stilben-4-yl)oxazole derives. XI (X1 = Ph) (X2, X3, % yield, and m.p. given): B, H, 76.8, 156-6.5.degree. (2); B2, H, 88.5, 204-5.degree. (5); B3, H, 86.0, 191.5-2.5.degree. (5); B6, H, 86.5, 142-2.5.degree. (2); B1, H, 80.1, 230-30.5.degree. (5); B4, H, 88.0, 169-9.5 (11); B5, H, 89.0, 214.5-15.degree. (11); B, Ph, 85.1, 181.5-82.degree. (5); B2, Ph, 84.0, 206-7.degree. (5); C6H4CH: CHC6H3Cl2-1,3, Ph, 55.6, 171.5-72.degree. (2); B3, Ph, 69.0, 182.5-83.degree. (5); B1, Ph, 92.5, 255-5.5.degree. (5) (XX); B4, Ph, 87.1, 159.5-60.degree. (2/3); B5, Ph, 86.2, 202-2.5.degree. (5); XI (X1 = X2, X3, % yield, and m.p. given): B1, Ph, 93.6,319-19.5.degree. (5); B, Ph, 70.1, 233-3.5.degree. (11); B4, Ph, 88.5, 242.5-43.degree. (11); B, B, 88.9, 239.5-42.degree. (5); B1, B1, 93.0, 274-5.degree. (5); the 2-(stilben-4-yl)thiazole and thiadiazole derivs. XII (X1, X2, Z, % yield, and m.p. given): Ph, B,:CH, 87, 210-10.5.degree. (11); Ph, B1,:CH, 93.5, 279-81.degree. (11); Ph, B,:N, 84.7, 227.degree. (5); Ph, B1,:N, 91.3, 320-20.5.degree. (7); C1, B,:N, 93.3, 317-18.degree. (7); C1, B1,:N, 95.0, 371-3.degree. (7); the following 5-stilbenzyl-1,2,4-oxadiazole derivs. VI (X1, X2, % yield, and m.p. given): Ph, B, 54.2, 144-4.5.degree. (2); Ph, B1, 70.0, 230-30.5.degree. (11); p-MeC6H4, B, 71.0, 158-9.degree. (2); p-MeC6H4, B1, 90.0, 294.5-95.degree. (11); the following stilbenzyl-1,3,4-triazole derivs. V (X = N) (X,X1, X2, % yield, and m.p. given): Ph, B, B, 90, 343-4.degree. (7); Ph, B1, B1, 88.7, >380.degree. (7); B, Ph, B, 96.5, 268-8.5.degree. (6); B1, Ph, B1, 85.6, 296-7.degree. (7); B, B, B, 92.5, 276-6.5.degree. (4); B1, B1, B1, 95.5, 365-6.degree. (7); B2, B2, B2, 87.8, 279.5-80.5.degree. (11); B3, B3, B3, 95.2, 260-60.5.degree. (7); B5, B5, B5, 95.5, 296.5-97.degree. (11); B4, B4, B4, 92.4, 319-19.5.degree. (7); the compds. XIII (X1, X2, X3, % yield, and m.p. given): B, B, Ph, 91, 219.5-20.degree. (11/10); B1, B1, Ph, 90.5, 315-17.degree. (4); the following stilbenylpyrazole derivs. XIV (X1, X2, X3, % yield, and m.p. given): B, Ph, Ph, 89.8, 164.5-65.degree. (ligroine); B1, Ph, Ph, 99.0, 212-13.degree. (10/11); Ph, B, Ph, 93.0, 216-16.5.degree. (10/11); Ph, B1, Ph, 17.0, 277.5-78.degree. (11); Ph, Ph, B, 90, 163.5-64.degree. (10); Ph, Ph, B1, 95.7, 208.5-209.degree. (2/4); B, B, Ph, 88.7, 236-7.degree. (11); B1, B1, Ph, 80.9, 318-19.degree. (11); the following stilbenylimidazole derivs. XV (X1, X2, % yield, and m.p. given): Ph, B1, 58.2, 308-8.5.degree. (7); Ph, B, 44.7, 253-3.5.degree. (5); Ph, B4, 70.3, 230.5-31.5.degree. (2/3); B1, Ph, 54.5, 226.5-27.degree. (5); B, B, 63.8, 234.degree. (2/3); B1, B1, 73.7, 285.5-86.degree. (11); Ph, 53.4, 274.5-75.degree. (11); the following stilbenylpyridine derivs. XVI (X1, X2, X3, % yield, and m.p. given): Ph, B, Ph, 59.8, 177.5-78.degree. (2/3); Ph, B1, Ph, 84.5, 275-275.5.degree. (4); B, Ph, B, 77.1, 256-7.degree. (10-11);

B1, Ph, B1, 86.6, 370-1.degree. (4); B, B, B, 93.8, 194.5-95.degree. (5); B1, B1, B1, 96.3, 347-50.degree. (7/4); the following stilbenylpyrimidine derivs. XVII (X1, % yield, and m.p. given): B, 79.5, 247-8.degree. (11); B1, 97.5, 345.5-7.5.degree. (7/4); B4, 97.4, 288-8.5.degree. (5/11); B5, 100.0, 281-1.5.degree. (7); the following styryl- and stilbenylquinoxaline derivs. XVIII (X1, X2, % yield, and m.p. given): H, A1, 94.4, 230.5-31.degree. (5); H, A, 84.3, 153.5-54.degree. (2); A, H, 93.0, 243.5-44.degree. (5); A1, H, 97.7, 321-3.degree. (7); A, A, 94.6, 300-2.degree. (11); A1, A1, 99.0, 350-3.degree. (5); the compds. XIX where X1 = X2 = p-C6H4N:CHQ(Q = 2-thienyl), yield 94.0%, m. 272.5-3.5.degree. (7) and where X1 = H and X2 = p-C6H4CH:CHQ (Q = 2-thienyl), yield 44.2%, m. 216-16.5.degree. (2); 2-[4-diethylaminostilben-1-yl]-4,5diphenyloxazole, 82.7, m. 198.5-99.degree. (3/2); the compd. XX yield 63.5%, m. 288-8.5.degree. (7). XI (X1 = X2 = Ph, X3 = p-MeC6H4) (7.78 g.) and 6.45 g. diphenylyl-4-carboxaldehyde anil in 200 ml. dimethylformamide were reacted with the exclusion of air in the presence of various alkali metals, the product cooled to room temp., 400 ml. aq. HCl added to acidic reaction, filtered, washed to neutral reaction with H2O and further purified by washing with 500 ml. MeOH, dried, and recrystd. from tetrachloroethene with the use of diatomaceous earth to yield XII. The results obtained were (alkali metal compd. in g., reaction period in min., temp., and m.p., and yield % given): LiNH2, 6.9, 60, 228-35.degree., 40; NaOH, 12.0, 120, 239-44.degree., 54; NaNH2, 11.7, 120, 249-51.degree., 68.3; NaOMe, 16.2, 90, 249-9.5.degree., 62.4; NaOMe, 16.2, 60, 253.5-54.degree., 86.8; KOH + 10% H2O, 12.5, 300, 252-2.5.degree., 75.0; KOH + 10% H2O, 12.5, 120, 253-3.5.degree., 83.5; KOH + 10% H2O, 12.5, 30, 254-4.5.degree., 88.4; KOH + 10% H2O, 12.5, 60, 254-4.5.degree., 85.2; KOCMe3, 8.41, 120, 253.5-54, 89.3; RbOH-2H2O, 10.0, 90, 254-4.5.degree., 81.3; CsOH.H2O, 10.0, 90, 253.5-54.degree., 83.5. The products prepd. are used as intermediates in the prepn. of dyes or pharmaceuticals and various products are suitable fluorescent brightening agents for synthetic org. materials of high mol. wt. such as homo- or copolymers, polycondensation products, poly addn. products, semi-synthetic org. materials, and natural org. materials. Examples of workup with Dacron, polyester granular of terephthalic acid ethylene glycol polyester, hexamethylenediamine adipate polyamide, and polypropylene are described. 16155-78-5P 16155-79-6P 16155-80-9P 16155-81-0P 16155-82-1P 16155-83-2P 16155-84-3P 16155-85-4P 16155-86-5P 16155-87-6P 16155-88-7P 16155-89-8P 16476-98-5P (prepn. of) 16155-78-5 HCA

1,3,5-Triazine, 2-[4-[2-(4-methoxyphenyl)ethenyl]phenyl]-4,6-

diphenyl- (9CI) (CA INDEX NAME)

IT

RN

CN

RN 16155-79-6 HCA CN 1,3,5-Triazine, 2-[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-4,6diphenyl- (9CI) (CA INDEX NAME)

RN 16155-80-9 HCA CN 1,3,5-Triazine, 2-phenyl-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-81-0 HCA

CN 1,3,5-Triazine, 2-[4-(1,1-dimethylethyl)phenyl]-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-82-1 HCA

CN 1,3,5-Triazine, 2-[1,1'-biphenyl]-4-yl-4,6-bis[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-83-2 HCA

CN 1,3,5-Triazine, 2,4-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-6-phenyl- (9CI) (CA INDEX NAME)

RN 16155-84-3 HCA

CN 1,3,5-Triazine, 2,4-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-6-[4-(1,1-dimethylethyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-85-4 HCA

CN 1,3,5-Triazine, 2-[1,1'-biphenyl]-4-yl-4,6-bis[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-86-5 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-(2-phenylethenyl)phenyl]- (9CI) (CA INDEX NAME)

RN 16155-87-6 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-(2-[1,1'-biphenyl]-4-ylethenyl)phenyl]-(9CI) (CA INDEX NAME)

RN 16155-88-7 HCA CN 1,3,5-Triazine, 2,4,6-tris[4-[2-(4-chlorophenyl)ethenyl]phenyl]-(9CI) (CA INDEX NAME)

RN 16476-98-5 HCA
CN 1,3,5-Triazine, 2,4,6-tris[4-(2-[1,1'-biphenyl]-4-ylethenyl)-2methylphenyl]- (9CI) (CA INDEX NAME)

```
C07D
IC
CC
     28 (Heterocyclic Compounds (More Than One Hetero Atom))
ST
     OXAZOLES BENZO; FLUORESCENT BRIGHTENING AGENTS; PYRIDINES;
     OXADIAZOLES; PYRIMIDINES BENZO; NAPHTHOTRIAZOLES; TRIAZINES;
     TRIAZOLES NAPHTHO; BENZOPYRIMIDINES; BENZOOXAZOLES
IT
     1552-56-3P
                   2718-87-8P
                                3962-65-0P
                                              6660-87-3P
                                                            6660-89-5P
     10165-24-9P
                   10307-62-7P
                                  14016-18-3P
                                                 14607-84-2P
                                                                16143-02-5P
                   16143-04-7P
     16143-03-6P
                                  16143-05-8P
                                                 16143-07-0P
                                                                16143-08-1P
     16143-09-2P
                   16143-10-5P
                                  16143-11-6P
                                                 16143-12-7P
                                                                16143-14-9P
     16143-15-0P
                   16143-16-1P
                                  16143-17-2P
                                                 16143-18-3P
                                                                16143-19-4P
     16143-20-7P
                   16143-21-8P
                                  16143-22-9P
                                                 16143-23-0P
                                                                16143-24-1P
     16143-25-2P
                   16143-26-3P
                                  16143-27-4P
                                                 16143-28-5P
                                                                16143-29-6P
                                  16143-33-2P
                                                 16143-34-3P
     16143-31-0P
                   16143-32-1P
                                                                16143-35-4P
     16143-36-5P
                   16143-37-6P
                                  16143-40-1P
                                                 16155-61-6P
                                                                16155-62-7P
     16155-63-8P
                   16155-64-9P
                                  16155-65-0P
                                                 16155-66-1P
                                                                16155-67-2P
     16155-68-3P
                   16155-69-4P
                                  16155-71-8P
                                                 16155-72-9P
                                                                16155-73-0P
                                                 16155-77-4P
     16155-74-1P
                   16155-75-2P
                                  16155-76-3P
     16155-78-5P 16155-79-6P 16155-80-9P
     16155-81-0P 16155-82-1P 16155-83-2P
     16155-84-3P 16155-85-4P 16155-86-5P
     16155-87-6P 16155-88-7P 16155-89-8P
                                  16157-10-1P
                                                 16157-11-2P
                                                                16157-12-3P
     16155-90-1P
                   16155-91-2P
     16157-13-4P
                   16157-14-5P
                                  16157-15-6P
                                                 16157-16-7P
                                                                16157-17-8P
                   16157-19-0P
                                  16157-20-3P
                                                 16157-21-4P
                                                                16157-22-5P
     16157-18-9P
     16157-23-6P
                   16157-24-7P
                                  16157-25-8P
                                                 16157-26-9P
                                                                16157-27-0P
     16157-28-1P
                   16157-29-2P
                                  16157-30-5P
                                                 16157-31-6P
                                                                16157-32-7P
                                                 16157-36-1P
     16157-33-8P
                   16157-34-9P
                                  16157-35-0P
                                                                16157-37-2P
                   16157-39-4P
                                  16157-40-7P
                                                 16157-41-8P
                                                                16157-42-9P
     16157-38-3P
                   16157-44-1P
                                  16157-45-2P
                                                 16157-46-3P
                                                                16157-47-4P
     16157-43-0P
     16157-48-5P
                   16157-49-6P
                                  16157-50-9P
                                                 16157-52-1P
                                                                16157-53-2P
                   16157-56-5P
                                  16157-57-6P
                                                 16157-58-7P
                                                                16177-90-5P
     16157-55-4P
     16177-91-6P
                   16177-92-7P
                                  16177-93-8P
                                                 16177-94-9P
                                                                16177-95-0P
                                                 16177-99-4P
     16177-96-1P
                   16177-97-2P
                                  16177-98-3P
                                                                16178-00-0P
     16178-01-1P
                   16178-02-2P
                                  16178-03-3P
                                                 16178-04-4P
                                                                16178-05-5P
     16178-06-6P
                   16178-07-7P
                                  16178-08-8P
                                                 16178-09-9P
                                                                16178-10-2P
                                                 16178-14-6P
                                                                16178-15-7P
     16178-11-3P
                   16178-12-4P
                                  16178-13-5P
     16178-16-8P
                   16178-17-9P
                                  16178-18-0P
                                                 16178-19-1P
                                                                16178-20-4P
     16178-22-6P
                   16178-23-7P
                                  16178-24-8P
                                                 16178-25-9P
                                                                16178-26-0P
                                                 16178-33-9P
                                                                16178-34-0P
     16178-30-6P
                   16178-31-7P
                                  16178-32-8P
                                  16178-37-3P
     16178-35-1P
                   16178-36-2P
                                                 16183-96-3P
                                                                16183-97-4P
     16183-98-5P
                   16184-00-2P
                                  16184-01-3P
                                                 16184-02-4P
                                                                16184-03-5P
                                                 16184-10-4P
                                                                16184-12-6P
     16184-07-9P
                   16184-08-0P
                                  16184-09-1P
                   16184-16-0P
                                  16184-17-1P
                                                 16184-18-2P
                                                                16184-19-3P
     16184-14-8P
                   16184-21-7P
                                  16184-22-8P
                                                 16184-23-9P
                                                                16184-24-0P
     16184-20-6P
     16184-25-1P
                   16184-26-2P
                                  16184-27-3P
                                                 16219-26-4P
                                                                16219-27-5P
                                                 16256-11-4P
                                                                16256-12-5P
                   16253-68-2P
                                  16256-10-3P
     16253-65-9P
                                                 16263-18-6P
                                                                16263-19-7P
     16256-13-6P
                   16263-16-4P
                                  16263-17-5P
                                  16263-23-3P
                                                 16263-24-4P
                                                                16263-25-5P
     16263-20-0P
                   16263-22-2P
                                                 16263-30-2P
                                                                16325-02-3P
     16263-26-6P
                   16263-28-8P
                                  16263-29-9P
                                  16443-36-0P
                                                                16445-47-9P
     16325-03-4P
                    16325-04-5P
                                                 16445-42-4P
     16445-80-0P
                                  16445-95-7P 16476-98-5P
                   16445-81-1P
```

(prepn. of)

6568-89-4 HCA

methylphenyl) - (9CI) (CA INDEX NAME)

RN CN

```
ANSWER 27 OF 27 HCA COPYRIGHT 2003 ACS
65:39064 Original Reference No. 65:7329c-f 4,4'-Bistriazinylstilbenes.
     (CIBA Ltd.). NL 6512338 19660324, 23 pp. (Unavailable). PRIORITY:
     CH 19640923.
GI
     For diagram(s), see printed CA Issue.
AB
     The title compds. (I) which are valuable optical bleaching agents
     for polymeric substrates are prepd. by heating mixts. of S and
     substituted s-triazines contg. a p-tolyl group at 290-300.degree. or
     from (4-ClCOC6H4CH:)2 (II) and benzonitriles at 70-130.degree. in
     the presence of AlCl3 and subsequently heating the reaction products
     with NH4Cl. For example, a mixt. of 14.46 g. II, 30.9 g. PhCN, and
     200 ml. anhyd. o-C6H4Cl2 was treated with 13.3 g. anhyd. AlCl3,
     heated to 120.degree., treated with 10.6 g. NH4Cl, stirred for 15
    hrs. at 120.degree., cooled, neutralized, and the o-C6H4Cl2 steam
     distd. to give 24 g. I (X = H), fluorescent needles m.
     >390.degree. (o-C6H4Cl2). A melt of 64.7 g. 2,4-diphenyl-6-(4-
     tolyl)-s-triazine and 3.2 g. S was stirred for 45-60 min. at
     290-300.degree., cooled after the formation of H2S had stopped,
     dissolved in 100 ml. o-C6H4Cl2 and 100 ml. C2Cl4, and cooled to
     18.degree. to give 24 g. II. Other I were prepd. (X and m.p.
     given): p-Me, 374-6.degree.; p-tert-Bu, >420.degree.; p-MeO,
     306-7.degree.; p-Cl, 373-34.degree.; and m-Cl, 385-6.degree..
     Examples of the use of I for fluorescent brightening of
    polyester, polyamide, poly(vinyl chloride), and polyethylene are
     given.
IT
     6568-89-4, s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-
     di-p-tolyl- 6568-90-7, s-Triazine, 2,2'-(vinylenedi-p-
    phenylene) bis [4,6-bis(p-tert-butylphenyl) - 6568-91-8,
     s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(m-chlorophenyl)-
        6739-71-5, s-Triazine, 2,2'-(vinylenedi-p-
     phenylene) bis [4,6-bis(p-methoxyphenyl) - 6888-33-1,
     s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-diphenyl-
     6888-34-2, s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-
    bis(p-chlorophenyl)-
        (prepn. of)
```

1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-bis(4-

RN 6568-90-7 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(p-tert-butylphenyl)- (7CI, 8CI) (CA INDEX NAME)

RN 6568-91-8 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(m-chlorophenyl)-(7CI, 8CI) (CA INDEX NAME)

RN 6739-71-5 HCA

CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(p-methoxyphenyl)- (7CI, 8CI) (CA INDEX NAME)

RN 6888-33-1 HCA CN 1,3,5-Triazine, 2,2'-(1,2-ethenediyldi-4,1-phenylene)bis[4,6-diphenyl- (9CI) (CA INDEX NAME)

RN 6888-34-2 HCA CN s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(p-chlorophenyl)-(7CI, 8CI) (CA INDEX NAME)

IC C07D

CC 46 (Dyes)

IT Bleaching agents

(fluorescent or optical, 2,2'-(vinylenedi-p-phenylene)bis[4,6-diphenyl-s-triazine] derivs. as)

IT Bleaching agents

(**fluorescent** or optical, 7-amino-3-phenylcoumarin derivs, as)

IT 6568-89-4, s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6di-p-tolyl- 6568-90-7, s-Triazine, 2,2'-(vinylenedi-pphenylene)bis[4,6-bis(p-tert-butylphenyl)- 6568-91-8,
s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-bis(m-chlorophenyl)6739-71-5, s-Triazine, 2,2'-(vinylenedi-pphenylene)bis[4,6-bis(p-methoxyphenyl)- 6888-33-1,
s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6-diphenyl6888-34-2, s-Triazine, 2,2'-(vinylenedi-p-phenylene)bis[4,6bis(p-chlorophenyl)(prepn. of)